ANL-FRA-1996-5

Group Theory Applied to Boundary Value Problems

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operated by The University of Chicago
for the United States Department of Energy under Contract W-31-109-Eng-38

ANL-FRA-1996-5

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December 1996

Work Supported by
U.S. Department of Energy
Nuclear Energy Programs

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ABBREVIATIONS

TE - transport equation
DE - diffusion equation
FE - finite element
FD - finite difference
RM - response matrix

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ABSTRACT

Applications of group theory to reactor physics problems is reviewed. The review deals only with boundary value problems of elliptic operators, which seems to be the orphan of applied mathematics. The discussion first formulates some general features of the methods and introduces its applications to reactor physics problems. First the boundary value problems are formulated. The irreducible components (irreps) of the boundary possess remarkable properties and the solution to a given problem will inherit the properties of the irreps if the involved operators meet the formulated requirements. The results are applied to a translational invariant case. A numerical method is established to solve linear elliptic problems. The method provides an arbitrarily accurate solution even if the discretization is coarse. Practical applicability is proven by reactor physics applications, where good accuracy, stability can be observed.

I. INTRODUCTION

There is a recent interest in the application of group theory to boundary value problems. This may be motivated by several reasons. First of all, there is hope for utilizing group theory to work out effective massively parallel algorithms. Secondly, group theory has found a large number of successful applications both in physics and mathematics, but boundary value problems apparently fell out of the scope of the application of group theory. Several attempts have been made to apply group theory to the boundary value problem; there are some results but a breakthrough has not been achieved.

The present work aims at applying group theoretic considerations to reactor physics. As the reader will see, in that context, symmetry considerations appeared long ago, partly because some of the leading personalities in reactor physics also made a significant contributions to group theory as well. An important area of those investigations is in lattice theory, where the reactor core is assumed periodic. The methods applied in lattice theory show a close similarity to lattice theory of solid state physics. Reactor physics lattice theory developed in a pragmatic way with group theory appearing only from time to time. The problem of non-uniform lattices demanded new methods. There the lattice involves cells of different type, the geometry of each cell type is the same, but the material composition may be different. A survey of the large number of approximations used in this problem was given by Deniz.[11] From the works of Berna,[5] Bonalumi,[7] Deniz,[11] and Selengut,[42] it became clear, at the end of the seventies, that in the computations of heterogeneous lattices it is important how each cell "responds" to its different surroundings. Therefore, the cell was embedded into different, typical surroundings as a first approximation, its response was investigated. The most important and simplest was a "uniform" surrounding. The second most important surrounding was meant to account for the non-uniformity of the surrounding cells. Berna, Bonalumi and Maiorov[27] proposed to embed the cell into a "cosine like" surrounding to determine its diffusion coefficient. Laletin, lead by practical considerations, set up a number of typical surroundings, see Ref. [22], i.e. boundary conditions to characterize the cell properties. Later on, it became clear that those "typical surroundings", in the group theoretic context, are the irreducible components of the general boundary condition. Since then, codes have been written and have been

applied to routine calculations and the problem of heterogenous lattices seems to have been solved. This problem is discussed in Section III.

The application of group theory got an impetus during the period from the second half of the seventies to the first half of the eighties. The first application of group theory was to the finite element method and was due to A. Fässler;[14] and S. Pelloni[37] worked out a method for application to practical problems. Applications to coarse mesh solutions of the neutron diffusion equation began with the work of Makai,[28] Makai, and Arkuszewski.[29] In diffusion theory, symmetry considerations have helped to develop analytic solutions for both square and hexagonal nodes so that the only approximation in the theory concerns the boundary condition.

Although the past achievements of group theory in physics are not touched in the present work, they should not be left unmentioned. If a given equation, for example, is considered without boundary conditions, we may ask what are those transformations which leave the equation invariant. In physics, those transformations have lead to general conservation laws. Ovsiannikov's[36] and Sattinger's[40] books give the desired tools. If the transformations which leave the equation invariant are known, then the mathematical question arises: in which coordinate system will the solution take its simplest form? The selection of special coordinate systems for a given equation are is connected with symmetry transformations. That question is treated in Miller's book[34] and in Olver's monograph.[35] Group theory is the basis of relationships between many different disciplines of mathematics, see Olver[35] and Mackey.[26]

It is well known that group theory has divided the scientific community. Its successes in physics, chemistry and mathematics speak for themselves. Still, mostly among physicist there has been at times considerable opposition. Why bother with group theory if the same results can also be obtained by other means? Wigner[49-50] has given the answer to this question.[1]

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[1]In the foreword to the Hungarian edition[50] of his book, Wigner writes: "Today we still feel that if a rule can be obtained by invariance postulates then it is worth to derive it in this way. This view relies on two arguments. The first may be that the consequences of invariance principles are more transparent, and more general than most conclusions obtainable by any specific calculation."

The present work does not pretend to contribute to group theory. It rather intends to present applications of group theory to specific practical problems. The elements of group theory for application to boundary value problems are given in Appendix A. There are several notations in use for the irreducible representations, the present work follows the notation of Ref. [23]. The notation, standard in reactor physics problems, is given in Appendix B.

In general, bold letters denote operators. The equation under consideration is written as

$$\mathbf{A}\Phi(x) = 0 \tag{I.1}$$

where **A** is a linear, elliptic operator, the independent variable x is in a convex set V. **O** denotes symmetry transformation of the above equation, G denotes the group of symmetries of operator **A**. Thus, a symmetry transformation $O \in G$, if $\mathbf{AO} = \mathbf{OA}$. The matrix associated with **O** is denoted by O, and its elements are O_{ik}. The equation under consideration is not always homogeneous.

II. SYMMETRIES AND BOUNDARY VALUE PROBLEMS

In this Section, we formulate the general boundary value problem. It will be shown that when the operators in the boundary value problem possess certain properties, the general problem can be split into a set of subproblems. In this way, group theory leads to a computationally more efficient formulation of the problem, and, in addition, to each subproblem there can be ascribed a physical meaning.

Consider a linear operator **A** acting on the function space $L_2(V)$, where V is a symmetric convex region. We assume that there is at least one operator transforming V into itself. For a boundary condition problem, we assume linear operator **B** forms a function given on the boundary. The range of operator **A** includes V, the range of operator **B** includes the boundary ∂V. The relationship between the symmetries of a region V and those of an operator **A** (or **B**) are defined in Appendix A. Those symmetries form respective groups G_V, G_A and G_B. The boundary value

problem is then determined by BVP (V, **A**, **B**). We define the symmetry of the boundary value problem as follows.

Definition 1. A linear operator **O** is said to have the symmetry of the boundary value problem (V, **A**, **B**) if (a) **O** transforms V into itself; (b) **O** and **A** commute: **OA=AO** and (c) **O** and **B** commute: **OB=BO**.

According to Definition 1, the symmetry group of the problem (V, **A**, **B**) is the intersection

$$G = G_V \bigcap G_A \bigcap G_B \tag{II.1}$$

where G_V, G_A and G_B are the symmetry groups of V, **A** and **B**, respectively.

The symmetries of problem (V, **A**, **B**) form a group. That group may consist of a single element, the identity transformation, or of an infinite number of symmetries. This partly depends on operators **A** and **B**. In a number of cases it suffices to assure that **O** commutes with **A**, then it commutes with **B** as well. Often **B** is the identity transformation (Cauchy type problem) or the normal gradient (Neumann type problem), or the linear combination of those two problems. Most boundary value problems of reactor physics belong to one of these.

Definition 2. Operators **A** and **B** are called **familiar** if **B** is such that **OA = AO** implies **OB = BO**.

It is easy to see that Cauchy and Neumann boundary condition problems involve familiar operators. In the former, **B** is the identity operator.

Definition 3. The $[0,\pi/2n_F)$ interval is closed from the left and open from the right and is called the ground (where n_F is the number of faces of V).

The symmetries of the boundary condition problem BVP(V, **A**, **B**) suggest the application of group theoretic techniques. Depending on the problem, the symmetries may form, for example,

a discrete group or a Lie group. The symmetries can also be arranged into classes (or conjugacy classes in the language of Sternberg,[46] Ludwig and Falter),[25] to which the results of group representation theory apply. Thus, by means of projection operator (A.6), any function can be decomposed into functions transforming according to the irreducible representations (irreps). First, we investigate basic properties of the irreps.

According to projection operator (A.6), the irrep f_i of a function f is a linear expression of f taken at different points in the range of f. Consequently, if f is n times differentiable, so is the irrep f_i. Let $f_i(\theta)$ be given in the interval $\theta \in [0,\pi/2n_F)$. The direction $\theta=\pi/2n_F$ is a symmetry axis and the character table tells us that f_i is an eigenvector of each symmetry operator with the eigenvalue given in the i^{th} row of the character table and in the column corresponding to the symmetry, thus by applying a reflection through the face to f_i we can obtain the function f_i in the range $[0,n_F)$. Here [,) denotes an interval closed from the left and open from the right. Now, applying the rotational symmetry of V, the $f_i(\theta)$ function is obtained for the entire $[0, 2\pi]$ interval. When f_i is a component of a two dimensional representation, more care is needed because the components may transform into each other. Thus, we arrived at the following statement.

Lemma 1. If $f(\theta)$ belongs to C^n then its irreps $f_i(\theta)$ determined by (A.6) also belong to C^n. The irrep $f_i(\theta)$, $0 \le \theta \le 2\pi$ is uniquely given by its value in the ground $[0, \pi/2n_F)$.

The first question is if we have a decomposition of the boundary condition do we also have a decomposition of the solution? What can we gain by such a decomposition of the solution?

Basic Lemma. Let the problem

$$\begin{aligned} \mathbf{A}\phi &= 0 \quad \text{in } V \\ \mathbf{B}\phi &= f \quad \text{on } \partial V. \end{aligned} \tag{II.2}$$

be given, and the linear operators **A** and **B** be such that

(a) When f = 0, the only solution is $\phi = 0$, i.e. the homogeneous problem has only the identically zero function as solution.

(b) The null space of operator **B** is empty, i.e. if $\mathbf{B}\phi=0$ then $\phi=0$.

Then, if f transforms according to the i-th irreducible representation on the boundary, the solution transforms according to the i-th irreducible representation inside V.

Proof: Let $f = f_i$ be a one-dimensional irreducible representation and ϕ_i the corresponding solution. Then, for any symmetry **O** we have $\mathbf{O}f_i = \alpha_i f_i$. Applying **O** to the second equation and making use of the commutation of **O** and **B**, we get $\mathbf{OB}\phi_i = \mathbf{BO}\phi_i = \alpha_i \mathbf{B}\phi_i = \alpha_i f_i$. Applying **O** to the first equation, we get $\mathbf{OA}\phi_i = \mathbf{AO}\phi_i = 0$. Multiplying the first equation by α_i, and because **A** is linear, we also have $\mathbf{A}(\alpha_i\phi_i) = 0$. Thus, we have the following equations for $(\mathbf{O}\phi_i - \alpha_i\phi_i)$:

$$\begin{aligned} \mathbf{A}(\mathbf{O}\phi_i - \alpha_i\phi_i) &= 0 \quad \text{in V} \\ \mathbf{B}(\mathbf{O}\phi_i - \alpha_i\phi_i) &= 0 \quad \text{on } \partial V, \end{aligned}$$

but according to assumption (a), the only solution is $(\mathbf{O}\phi_i - \alpha_i\phi_i) = 0$, which proves the statement for a one-dimensional representation. Note that the second equation above is not true unless assumption (b) is met.

Let $f = f_i$ be a component of a two- or three-dimensional representation, i.e. it transforms as

$$\mathbf{O}f_i = \sum_k O_{ik} f_k .$$

The boundary condition (BC) for each component k is given by $\mathbf{B}\phi_k = f_k$. Multiplying that equation by O_{ik} and summing over k, **B** being linear, we have

$$\mathbf{B}\left(\sum_k O_{ik}\phi_k\right) = \sum_k O_{ik} f_k .$$

Multiplying the second equation of the problem by O, and using the linearity of **B**, we have

$$\mathbf{OB}\phi_i = \mathbf{BO}\phi_i = \sum_k O_{ik} f_k .$$

Subtracting the last two equations, we get by means of assumption (b)

$$\mathbf{B}\left(O\phi_i - \sum_k O_{ik}\phi_k \right) = 0 ,$$

thus on ∂V ϕ_i transforms as the i-th column of a multidimensional representation.

As to the transformation rules in V, if we multiply the first equation in (II.2) by O_{ik}, sum over k on one hand, and multiply the equation again by **O,** we have

$$\mathbf{A}\left(O\phi_i - \sum_k O_{ik}\phi_k \right) = 0 .$$

The last two equations form a BVP, the only solution of which is identically zero. This completes the proof. Certainly the second step of the proof also includes the first step.

Corollary. By virtue of the linearity of the problem, when a volumetric source Q is included the solution to

$$\mathbf{A}\Phi_Q = Q \text{ in } V$$
$$\mathbf{B}\Phi_Q = f \text{ on } \partial V$$

is given by $\Phi_Q = \Phi + \Psi$, where Φ is the solution of (II.2) and Ψ is the solution of

$$\mathbf{A}\Psi = Q \text{ in } V$$
$$\mathbf{B}\Psi = 0 \text{ on } \partial V .$$

Applying the argument used in the proof of the Basic Lemma, we arrive at the following result. Let q_i be the ith irreducible component of Q. Then an irreducible decomposition of Φ_Q is $\Phi_Q = \Psi_i + \Phi_i$, where

$$\mathbf{A}\Psi_i = q_i \text{ in } V$$
$$\mathbf{B}\Psi_i = 0 \text{ on } \partial V$$

and

$$\mathbf{A}\Phi_i = 0 \text{ in } V$$
$$\mathbf{B}\Phi_i = f_i \text{ on } \partial V.$$

The basic lemma allows one to find suitable representations for the boundary values on ∂V and for the solution in V. The general prescription is to find suitable representations, with which a general function, given along the boundary, is decomposed into irreps, and solve the above equations for the components. To this end the projector (A.6) is applied. We set forth the following notation. A point x on the ∂V boundary of the convex volume V is characterized by an angle θ measured from a suitable center inside V. We assume furthermore, that ∂V consists of n_F faces. When V is a regular triangle, square, hexagon or pentagon the faces are of equal length or area and there are $2n_F$ symmetry transformations leaving V invariant. Now the symmetries of the problem transform one point of the boundary into another boundary point. Thus the projector (A.7) applied to a function $f(\theta)$ will give linear combinations of $f(\theta_i)$, $i = 1, 2n_F$.

Lemma 2. The irreps of a boundary value $f(\theta)$ take the form

$$f_i(\theta) = g_i\left(\theta \bmod \pi/n_F\right) e_i\left(\left[\frac{\theta}{\pi} n_F\right]\right) \qquad \text{(II.3)}$$

where [ ] denotes the entire part, the function e_i assigns an integer number to its argument, and the g_i function is not identically zero on the ground.

Proof: Let us note that the $f_i(\theta)$ functions are orthogonal in the following sense:

$$\int_0^{2\pi} f_i(\theta)\, f_j(\theta)\, d\theta = \theta_{ij} \qquad \text{if } i \neq j \ .$$

Furthermore, any function can be expressed as a linear combination of functions $f_i(\theta)$. It suffices to show that there is a function e_i with which $f_i(\theta)$ transforms according to (**A**7). First, we note that the argument of e_i takes $2n_F$ values, thus, e_i may take at most $2n_F$ distinct values. Hence, e_i may be represented as a vector of $2n_F$ values. The components of the vector correspond to the intervals $(k-1)\pi/n_f \le \theta < k\pi/n_f$. Thus, finding functions e_i reduces to finding irreps in a $2n_F$ dimensional space which can be achieved by means of Eq. (A.6) by starting out from a suitable initial vector. The g_i function may not be identically zero on the ground, and has no influence on the symmetry properties of $f_i(\theta)$. Thus the lemma is proven.

As an illustration, Fig. 1 shows the $f_i(\theta)$ for a square shaped node. We assumed that $g_i = 1$. There are six irreducible components, four of them (A_1, A_2, B_1 and B_2) are one dimensional, and there are two equivalent two dimensional representations, (E_1 , E_2) and (E_3, E_4) which form a pair, respectively. The irreps are numbered in Fig.1 from bottom to top. The eight functions in Fig. 1 give the variation of the irreps on the eight half sides. The argument of $f_i(\theta)$ is the angle variable and each side covers a $\pi/2$ wide range. When g_i differs from unity, g_i modulates the i-th function e_i.

The above two lemmas form the basis of applying group theory to boundary value problems. The Basic Lemma states that if operators **A** and **B** have the required properties, the solution inside V will inherit the symmetry properties of the function prescribed on the boundary. That statement is remarkable, because the boundary ∂V is a simpler geometrical formation than the region V. It is noteworthy, that a precursor of Basic Lemma appeared first in 1982, see Ref. [30], notwithstanding that the first application of group theory to the boundary

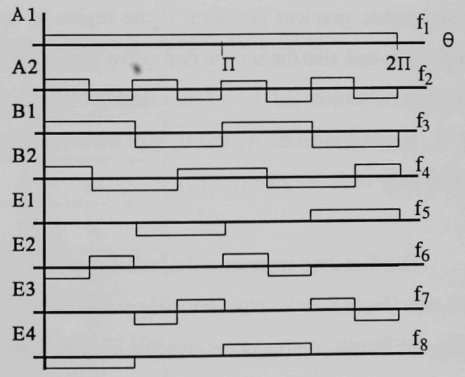

Fig. 1. Irreps on the Boundary of the Square (g_i=constant)

value problem is more than 40 years old, see (Stiefel, Ref. [47]). A possible explanation is that in many cases it is evident that the homogeneous problem has no nontrivial solution. In reactor physics, on the other hand, nontrivial solutions of the homogeneous problem are of major importance.

Lemma 2 is actually a trivial consequence of the properties of the irreducible components obtained by expression (A.6), but its importance justifies formulating it as an independent assertion. The e_i vectors bear important physical meaning which is apparent in simple geometries. In one dimension, for example, we have two components: $e_1 = (1,1)$; $e_2 = (-1,1)$. The first vector says that the left and right boundaries are equal. The second vector represents a gradient. A solution of any boundary value problem can be composed from the solution of a symmetric problem and of the antisymmetric gradient problem. If the region is more complex, the gradient may have more components and also the second derivative

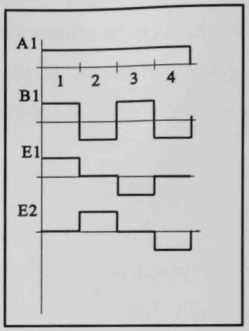

Fig. 2. Simplified Irreps on the Boundary of a Square

boundary value problem can be composed from the solution of a symmetric problem and of the antisymmetric gradient problem. If the region is more complex, the gradient may have more components and also the second derivative may appear. As an illustration, we present a simplified boundary condition (i.e. by a four element vector) prescribed on the boundary of a square, see Fig. 2. Representations A_2 and B_2 will be zero, and the two-dimensional representation will be present only with one pair (E_1, E_2).

The first irrep represents the homogeneous surroundings, the second irrep is a gradient along the x axis (faces 1 and 3 have normal parallel to the x axes), the third irrep is a gradient along the y axis, the fourth component represents a cross-flow, a kind of second derivative.

Let us decompose the $g_i(\theta)$ function into a power series:

$$g_i(\theta) = \sum_{k=0}^{N} c_{in}\theta^n \qquad \text{(II.4)}$$

where c_{in} are arbitrary coefficients. Retain the e_i functions as introduced in Fig.1, then the irreps in expression (II.3) involve the up to N-th order Walsh functions (Seed and Albrecht, Ref. [41]).

Consider the Fourier transform of $g(\theta)$. Because it is a periodic function with period 2π, in the Fourier series only the integer (k) components contribute:

$$g(\theta) = \sum_{k=0}^{\infty} a_k \cos k\theta + b_k \sin k\theta = \sum_{k=1}^{3} \sum_{m=1}^{\infty} \left(a_{4m+k} \cos(4m + k)\,\theta + b_{4m+k} \sin(4m + k)\epsilon \right.$$
$$= \sum_{k=0}^{3} E_k(\theta) + \Theta_k(\theta) \qquad \text{(II.5)}$$

with $b_0 = 0$. Those components for which k(mod n_F) is a given number, transform the same way under the symmetries of V, thus they are collected into one even ($E_k(\theta)$) and one odd ($\Theta_k(\theta)$) function. Table 1 gives the correspondence between those functions and the irreps.

Table I. Irreps and Fourier Components on a Square Boundary.

Fourier Component	Subspace
E_0	A_1
E_1	E_1
E_2	B_1
E_3	E_2
Θ_0	A_2
Θ_1	E_1
Θ_2	B_1
Θ_3	E_2

A model allows a formulation of relationships between two physical quantities given on the boundary. Let $f(\theta)$ and $h(\theta)$ be two given quantities on the boundary ∂V. Their relationship is given by the expression

$$h(\theta) = \int_0^{2\pi} G(\theta,\theta') f(\theta')d\theta' \qquad \text{(II.6)}$$

where G is a given function. Usually $h(\theta)$ and $f(\theta)$ are expanded into coordinate functions (i.e , functions of x and y). Of special interest are the coordinate functions which represent the values on the faces.

Definition 4. Let $\mathbf{h} = (h_1,...,h_{nF})$ and $\mathbf{f} = (f_1,...,f_{nF})$ the values of function h and f on the n_F faces. The matrix R joining **f** and **h** as

$$\mathbf{h} = \mathbf{Rf} \qquad \text{(II.7)}$$

is called a response matrix.

There are a number of response matrices depending on the f and h quantities. Most frequently f is the solution to an elliptic equation and h is constant times the normal derivative. Another important case is when their linear combinations are encountered, see Appendix B for details. In those cases, **R** commutes with the symmetries of V. To see this, we have to show that the normal gradient is invariant under a symmetry O. This is the case because according to Definition A.1 $O(\mathbf{n}\nabla) = (O\mathbf{n}O\nabla) = (\mathbf{n}\nabla)$, where n is the normal to the surface; because the symmetries are equivalent to unitary transformations (see Appendix A). Applying Schur's lemma (see Appendix A) to problem (II.2), we arrive at Lemma 4.

Lemma 4. If V is a symmetric region then any response matrix, as in Definition 4, is block diagonalized by expressing both **h** and **f** in the irreducible components.

Lemma 4 implies a rather positive statement, viz. if the response matrix is applied to a vector (input) transforming as a given component of an irrep, the response will keep the symmetry properties of the input. For example, in a regular hexagonal node, the response matrix connects 6 faces to 6 faces, whereas the 6 irreps do not mix.

The results of the present section is summarized as follows. If we have a group given, the solution space can be decomposed into irreducible, orthogonal subspaces. The decomposition is based on expression (A.6). If the given group commutes with the BVP, then the operators involved in the problem leave each subspace invariant. As a consequence, the decomposition into irreps on the boundary entails a decomposition inside the volume. Furthermore, any matrix that connects two types (e.g. flux and net current) of functionals formed from the solution with the help of **A** and **B**, will be diagonal. The above decompositions form the basis of the applications in the subsequent sections.

III. NON-UNIFORM LATTICES

Let us assume that among the symmetries of operator **A** we also have the translational symmetries given in two-dimensions by $n\,\mathbf{a}_1 + m\,\mathbf{a}_2$, where n, m are integers, $\mathbf{a}_1$ and $\mathbf{a}_2$ are so called elementary translations[10] bringing the lattice into itself. Then, the irreducible representations are eigenfunctions of the translational operator, the solution can be decomposed into irreps, and the results of Appendix A apply. A survey of reactor physics lattice theory is given in Ref. [11]. The lattice, however, is an abstraction. Every real structure is finite, even if its internal structure is a repetition of an element called a cell.

Definition 1. The cell is the elementary unit of volume V.

Definition 2. The lattice obtained by repeating a single cell type is called homogeneous lattice. The lattice containing more than one cell types is called non-uniform lattice.

Translational symmetries can be exploited when solving the neutron transport (or diffusion) equation in the same manner as in solid state physics. That fact has been known for a long time, still, in reactor physics, the first systematic study appeared in 1974 in Ref. [6]. A more recent survey has been given by Deniz.[11] In these studies every lattice is finite; furthermore, there are irregularities in the lattice (e.g. a cell is filled out by structural or absorber material) and which need to be taken into account. Below a brief summary is given on the application of the results of Section II. to the theory of finite lattices.

Let us first consider a given linear operator **A** over an infinite lattice. If $\mathbf{A} + k^*\mathbf{d}) = \mathbf{A}(\mathbf{r})$ for any integer k and for a lattice vector **d**, then $\mathbf{AT}(k^*\mathbf{d}) = \mathbf{T}(k^*\mathbf{d})\mathbf{A}$, where **T** is the translation operator. Thus, the symmetries of **A** include translation as well. The technique of exploiting the translational symmetry has been demonstrated some time ago (see for example, Callaway, Ref. [10]). An application to the formalism of reactor physics is given in Ref. [31]. From technical point of view, the lattice is a special discretization of a volume, where the identical subvolumes are called cells.

In the present Section, we apply the group theoretic results in Appendix A to the solution of the neutron transport equation (TE), Eq. (B.5). The basic terms of neutron physics are briefly summarized in Appendix B. The results of the application to the analysis of the TE can be summarized as follows:

1. The irreps of the neutron transport equation in a homogeneous lattice are the Bloch's functions:[10, 11]

$$f_B(\mathbf{x}) = f_B(\mathbf{r},E,\Omega) = e^{iBr}u_B(\mathbf{r},E,\Omega)$$

where $u_B(\mathbf{r},E,\Omega) = u_B\mathbf{r} + n^*\mathbf{a}_1 + m^*\mathbf{a}_2, \Omega)$.

2. The eigenfunctions of the transport operator **A** can be expressed by Bloch's functions

$$\Phi(x) = \sum_{B} c(B) * e^{iBr} u_B(x) \qquad \text{(III.1)}$$

where c(**B**) are arbitrary coefficients.

3. The periodic part of the Bloch's function satisfies the equation

$$\mathbf{A}(u_B)e^{iBr} = -\mathbf{A}(e^{iBr}) * u_B \qquad \text{(III.2a)}$$

where $\mathbf{A}(e^{iBr} * u_B) = \mathbf{A}(e^{iBr}) * u_B + \mathbf{A}(u_B)e^{iBr}$. Furthermore, u_B possesses the following symmetries:

$$u_{OB}(\mathbf{x}) = u_B(O^{-1}\mathbf{x}) \qquad \text{(III.2b)}$$

i.e. the periodic part of Bloch's function associated with vector **OB** (left hand side of Eq. (III.2b)), is the same as the function $\mathbf{O}u_B$ (the right hand side of Eq. (III.2b)). See Definition A.1.

4. The Bloch's functions are orthogonal in the following sense:

$$\left(f_B^{+}, f_{B'}\right) = 0 \quad \text{if } \mathbf{B} \neq \mathbf{B}.$$

Here $f_B = e^{iBr} * u_B(x)$ and the bracket denotes integration over x and superscript + refers to complex adjoint.

5. Integrals of the type

$$\left(f_B^{+}; \mathbf{A} * f_{B'}\right) = \int d\mathbf{r} d\Omega dE f_{B'}(\mathbf{r},E,\Omega)\mathbf{A} * f_B(\mathbf{r},E,\Omega)$$

are zero unless f_B^{+} and f_B belong to the same invariant subspace, c.f. Theorem (A.2).

6. Expanding the periodic part in Bloch's function into a Taylor series around $\mathbf{B} = 0$,

$$u_B(x) = u_0(x) + \sum_j u_{1j}(x)B_j + \ldots \qquad \text{(III.3a)}$$

We get the following expressions for the eigenfunctions:

$$\Phi(x) = \left(\sum_B e^{iBr}\right) u_0(x) + \sum_j \left(\sum_B e^{iBr} iB_j\right) u_{1j}(x) + \ldots \qquad \text{(III.3b)}$$

We note here, that the decomposition (III.3a) of the periodic part of Bloch's function facilitates the determination of the irreps of u_B. Using the projector (A.6) and property (III.2a), we see that u_0 is the irrep transforming as the unit representation, u_{1j} are components of a two dimensional representation. At the same time, the irreps have a physical meaning, $u_0(x)$ is the solution of Eq. (I.1) in the infinite periodic lattice, $u_{1j}(x)$ is an odd periodic function to be determined from (III.2). In Eq. (III.3b), the first term in brackets is called in neutron physics the macroflux. We note that expression (III.3) expresses the solution in a finite lattice, whenever the macroflux satisfies the boundary condition prescribed at the surface of the finite lattice.

The above derivation based on different assumptions has been known for a long time. Below it is extended to non-uniform lattices, i.e. to cases where the geometry of the cells is identical but the internal structure, the material distribution may vary from cell to cell. Also a new derivation of an asymptotic form to the neutron transport equation will be given. The TE is described in Appendix B.

In a non-uniform lattice, the eigenfunctions of the TE (III.3a) can be generalized by expanding them into irreducible components on the cell boundary. When the cells are small, average entering

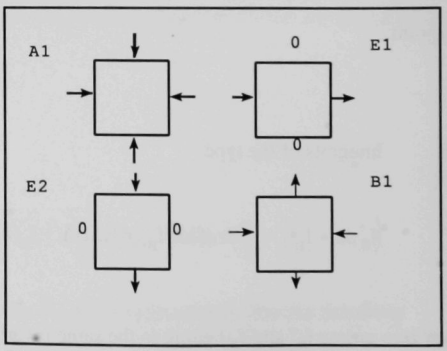

Fig. 3. Irreducible Entering Current Patterns for Square Cell

currents may be prescribed on the cell boundary. In a square cell, the decomposition of the boundary flux into irreps results in A_1, B_1, E_1 and E_2 terms, see Fig. 2. According to the Basic Lemma, if the cell is sufficiently small, this decomposition induces a decom-position inside the cell. The solution to the transport equation with irreducible boundary condition is considered as a response to the boundary condition. The entering current patterns are given in Fig. 3.

The A_1 term of the solution corresponds to u_0 and describes the cell response when imbedded in homogeneous surroundings, the E_1 and E_2 terms describe the cell responses when imbedded it into an x and y directed gradients, respectively. The B_1 term describes the cross-flow. Because any boundary condition can be decomposed into irreps, the above cell responses exhaustively characterize the cell. Hence, the solution to the TE can be written as

$$\Phi(x) = X_1 * u_1(x) + X_2 * u_2(x) + X_3 * u_3(x) + X_4 * u_4(x) \qquad \text{(III.4)}$$

where each X_i is a constant in a cell, whereas each $u_i(x)$ is a solution to the TE in the cell. We are able to calculate the exiting current from the $u_i(x)$ functions and arrive at a decomposition of the exiting current at the boundary. This expression involves response matrices determined from the u_i functions. Let the numbering of the irreps in Eq. (III.4) be the following. Subscript i = 1 corresponds to the symmetric A_1 term, the response matrix determined from u_1 being r_1. Indices i = 2 and 3 correspond to terms E_1 and E_2, with one common response matrix r_2. This is because the cell is assumed to be symmetric, hence the x and y directions must be identical. The fourth term correspond to B_1, with response matrix r_3.

It can be shown, following Ref. [22] and Ref. [32], that the continuity of the partial currents at cell boundary leads to a finite difference equation for X_1. For this, we make the following assumption.

Assumption 1. We assume the cells have different r_1 matrices, but identical r_2 and r_3 matrices.

For the derivation of an equation for X_l, we introduce a cell index, and number the cells. The cell numbering scheme is shown in Fig. 5. In cell No. j, X_{lj} is the A_l term of the entering current, r_{lj} is the RM of the A_l component $u_{lj}(x)$ etc. The angular entering current depends on the angular variable Ω. To account for that dependence, each partial current is replaced by its first Legendre components:

$$X_{kj} = X_{kj}^{(0)} + \mathbf{X}_{kj}^{(1)}\Omega + \ldots \qquad \text{(III.5)}$$

where $X_{kj}^{(0)}$ is scalar, but $\mathbf{X}_{kj}^{(1)}$ is a vector (cf. Eq. (B.6)-(B.7)) and transforms accordingly. The continuity of partial currents is assured by the continuity of $X_{kj}^{(0)}$ and $X_{kj}^{(1)}$, the latter takes opposite signs at the two sides of a node surface.

The $X_{lj}^{(0)}$ term is given by

$$X_{10}^{(0)} = \left(\sum_{j=1}^{4} \sum_{k=1}^{4} e_{jk} X_{kj}^{(0)} \right) . \qquad \text{(III.6)}$$

X_{10} is the average of the entering currents at the four faces. The first term of the entering current is continuous at a given face, and is reconstructed from the irreps of the neighboring nodes multiplied by the adjoint of matrix **E**. This matrix is formed from

$$\mathbf{E} = \begin{pmatrix} \mathbf{e}_1/2 \\ \mathbf{e}_2/2 \\ \mathbf{e}_3/\sqrt{2} \\ \mathbf{e}_4/\sqrt{2} \end{pmatrix} . \qquad \text{(III.7)}$$

The step functions $\mathbf{e}_i$ are given in Fig. 2. The continuity of the first moments is specified by

$$\mathbf{R}_{10}X_{10}^{(0)} = \sum_{j=1}^{4}\sum_{k=1}^{4}\left(\mathbf{R}_{kj}X_{kj}^{(0)}\right), \qquad \text{(III.8)}$$

where the RMs R_{kj} and r_{kj} are related by

$$\mathbf{R}_{kj} = \frac{1}{2}(r_{kj} - 1)(1 + r_{kj})^{-1} .$$

According to Assumption 1, $R_{2j} = R_{3j} = R_2$. Multiplying Eq. (III.6) by R_{10} and subtracting (III.8), we get

$$\frac{1}{h^2}\sum_{j=1}^{4}(\Psi_j - \Psi_0) - \mathbf{B}_0^2\Psi_0 = \frac{1}{h^2}(\mathbf{R}_2 - \mathbf{R}_4)\sum_{k=1}^{4}X_{4j}\mathbf{e}_{4j} . \qquad \text{(III.9)}$$

Here the matrix B_j is given by

$$\mathbf{B}_j^2 = \frac{8}{h^2}\mathbf{R}_2\left(\mathbf{R}_{1j} - \mathbf{R}_2\right)^{-1}$$

and

$$\Psi_j = (R_{1j} - R_2) * X_{1j}^{(0)}.$$

Usually the fluxes are positive numbers of equal magnitude, thus, X_{4j} is often negligible. Then (III.9) is the finite difference form of the diffusion equation. What we obtained, is an asymptotic form of the transport equation valid for a finite mesh size h. Although it is off the main thrust of the present work, we remark that it is possible to derive a generalized diffusion coefficient by means of the above considerations. Details are given by Gadó et al. in Refs. [15] and [12]. A similar decomposition holds in hexagonal and triangular lattices as well.

IV. A NUMERICAL METHOD

1. Formulation of the Method

The proposed approximation is applied to the solution of the diffusion equation, see Appendix B. Consider the following problem.

$$\begin{aligned} \mathbf{A}(k)\Phi(x) &= 0, \text{ in } V \\ \mathbf{B}\Phi(x) &= 0 \text{ on } \partial V \end{aligned} \tag{IV.1}$$

where $\mathbf{A}(k)=\mathbf{A}_1+1/k*\mathbf{A}_2$ and V is convex and composed of homogeneous regions:

$$V = \bigcup_{j=1}^{N} V_j \tag{IV.2}$$

where regions j and j' are disjoint except the joint boundary $\partial V_{jj'}$. N is the number of homogeneous regions. Let ∂V_j denote the boundary of region (or node) j, then

$$V_j \bigcap V_{j'} = \partial V_{jj'} = (\partial V_j) \bigcap (\partial V_{j'}) . \tag{IV.3}$$

A boundary ∂V_j is called external boundary, if

$$\partial V_j \bigcap \partial V = \partial V_j . \tag{IV.4}$$

If ∂V_j is not external, then it is an internal boundary. $\mathbf{A}(k)$ and $\mathbf{B}$ are linear operators. Both $\mathbf{A}(k)$ and $\mathbf{B}$ may involve functions as coefficients. Furthermore, $\mathbf{A}(k)$ be such that the Krein-Rutmann theorem[21] holds. That is, $\mathbf{A}$ is a positive compact operator on a Banach space of functions with a cone C of non-negative functions such that for some $x \in C$, $\alpha>0$ and a positive integer n, for which

$\mathbf{A}^n x - \alpha x \in C$.

In volume j the equation to be solved is written as

$$\mathbf{A}_j \Phi_j(x) = 0 , \tag{IV.5}$$

where subscript j refers to region j in which the coefficients associated with each $\mathbf{A}_j$ may be different. We assume, furthermore, the existence of a value of parameter k which turns the largest eigenvalue of **A**(k) into zero. The associated eigenfunction is nonnegative. We seek the solution of BVP (**A**, **B**,V). Such problems have been addressed in physics, see Refs. [19, 43].

There is only one assumption for the proposed numerical method.

Assumption. It is sufficient to ensure the continuity of face averages of the solution and its gradients on internal boundaries. Let $\partial V_{jj'}$ denote the joint boundary of volumes j and j'. Then, with D_j, j = 1,N, given, the assumption is explicitly expressed as

$$\begin{aligned} \int_{\partial V_{ij}} \Phi_i(x) dF_{ij} &= \int_{\partial V_{ij}} \Phi_j(x) dF_{ij} \\ -D_i \int_{\partial V_{ij}} \partial_n \Phi_i(x) dF_{ij} &= D_j \int_{\partial V_{ij}} \partial_n \Phi_j(x) dF_{ij} . \end{aligned} \tag{IV.6}$$

On external boundaries operator **B** involves only linear expressions of face averages:

$$\mathbf{B}\Phi = a_j \int_{\partial V_j} \Phi_j(x) dF_j + b_j \int_{\partial V_j} \partial_n \Phi_j(x) dF_j = 0 \tag{IV.7}$$

The stipulated features of operator **A**(k) permit the application of the Krein-Ruttmann theorem. Thus, there exists an eigenvalue of **A** which is positive and the associated eigenfunction is also positive. The proposed numerical method exploits these properties.

Definition 1: The function

$$e^{ibx}F_j(b) \tag{IV.8}$$

where $F_j(b) \neq 0$ is the Fourier transform of $\Phi(x)$, is called an **elementary solution** to Eq. (IV.1). Note that an elementary solution meets the first equation of problem (IV.1), but not the boundary condition.

Remark. When the coefficients in operator **A** are constant in space, the elementary solution is obtained by Fourier transforming the first equation in problem (IV.1). The transform will be a polynomial of b multiplied by F(b).

Proposition 1. Let **O** be a symmetry of the BVP (**A**, **B**, V). Then $F_j(\mathbf{O}b) \neq 0$ provided $F_j(b) \neq 0$.

Proof: If **O** is a symmetry and e^{ibx} is an elementary solution, then $e^{i(Ob)x}$ is also an elementary solution.

In the elementary solution, $F_j(b)$ can be dropped since it is only a constant multiplier.

With the help of the elementary solutions, the following trial function is composed

$$\Phi_j(x) = \sum_{k=1}^{n_F} c_{jk}(b_k)e^{ib_kx} . \tag{IV.9}$$

The notation $c_{jk}(b_k)$ indicates that, through index *k*, the "*c*" is connected to a "*b*" value of the Fourier transform of the solution. Here (c_{jk}, k = 1,...,n_F) denote free constants that need to be determined. The above trial function satisfies the first of Eq. (IV.1) inside V_j. The proposed trial function involves n_F*N unknowns c_{jk} over V. The internal and external boundary conditions involve the same number of equations. The equations are linear in the undetermined constants c_{jk}. Whether a given equation is solvable or not that depends on the properties of the matrix of the equation. When either the first equation or the second in Eq. (IV.1) is non-homogeneous and the matrix is not singular, the c_{jk} coefficients can be determined. If the problem is homogeneous, the solution exists only if the matrix is singular. This can be assured under the stipulated conditions by setting k so that the largest eigenvalue of operator **A** is zero. To do so, we need the following property of the eigenvalue of operator **A** (see Ref. [8]).

Lemma 1. The largest eigenvalue of operator **A** is a monotone function of k and tends to infinity as k tends to zero.

Proof: Let $\alpha(k)$ be the largest eigenvalue of **A**. The largest eigenvalue equals the spectral radius of **A**:

$$\alpha(k) = \lim_{n\to\infty} \|\mathbf{A}^n(k)\|^{\frac{1}{n}} .$$

Take two different values of k, say k_1 and $k_2 > k_1$. We then have

$$\alpha(k_1) = \lim_{n\to\infty} \|\mathbf{A}^n(k_1)\|^{\frac{1}{n}} \geq \lim_{n\to\infty} \frac{\|\mathbf{A}(k_1)^n\Psi(k_2)\|^{\frac{1}{n}}}{\|\Psi(k_2)\|} \geq \lim_{n\to\infty} \frac{\|\mathbf{A}(k_2)^n\Psi(k_2)\|^{\frac{1}{n}}}{\|\Psi(k_2)\|} = \alpha(k_2) .$$

This proves the monotonicity of $\alpha(k)$. Now let k tend to zero. In the eigenvalue problem

$$\mathbf{A}(k)\Psi = \alpha(k)\Psi \qquad \text{(IV.10)}$$

the left hand side is the sum of two terms, one of them is independent of *k*, the other is proportional to *1/k* and tends to infinity. The eigenfunction can always be normalized. Thus, $\alpha(k)$ tends to infinity as k tends to zero. By means of the Shmulian theorem,[44] we get that $\alpha(k)$ may not be constant for an interval of positive measure, thus, $\alpha(k)$ is a strictly decreasing function.

This lemma suggests an iteration scheme. Starting from a k_0 value, we derive elementary solutions and combine them as given by (IV.9). We can estimate the largest eigenvalue of $\mathbf{A}(k_0)$, and if it is positive (negative), the next estimate for k will be $k_0 + \Delta k$ ($k-\Delta k$), with $\Delta k>0$. Starting from a positive k_0 and a positive initial guess of Φ, an approximate solution can be given. The solution is more effective, if the following tricks are introduced. The existence of the largest eigenvalue and associate eigenvector can be translated into another eigenvalue problem, and the associated matrix can be simplified by means of group theoretic considerations.

First, at the boundary two linear combinations are formed from the averages of the solution and of its normal gradient. The response matrix connecting the two linear combinations is calculated from the trial function (IV.9), and the continuity conditions (IV.6)-(IV.7) yield an eigenvalue problem. That eigenvalue problem is solved in a two level iteration. At the first level we determine the largest eigenvalue of a matrix depending on parameter k, at the second level the parameter is set so that the largest eigenvalue be unity.

Definition 2. Let x be on an external or internal boundary. The following linear combination of the solution and a given positive constant (D) times its normal gradient is called an entering current (J^-):

$$J^-(r) = \frac{1}{4}\left(\Phi(x) + 2D\partial_n\Phi(x)\right). \qquad \text{(IV.11a)}$$

The constant D belongs to that volume V_i, from which the normal n is outward.

Definition 3. The following linear combination of the solution and a given positive constant (D) times its normal gradient is called entering current (J^+):

$$J^{+}(r) = \frac{1}{4}\left(\Phi(x) - 2D\partial_n\Phi(x)\right). \qquad \text{(IV.11b)}$$

Definition 4. The operator **F** and **E** form the face averaged flux and net current respectively, and are given by

$$\mathbf{E}*\Phi(x) = \int_F \Phi(x)dF; \quad \mathbf{F}*\Phi(x) = \int_F \partial_n\Phi(x)dF \ . \qquad \text{(IV.12)}$$

In accordance with Assumption 1, it suffices to prescribe face averaged gradients and fluxes on the boundary. Thus, the average entering and exiting currents on surface i of node j given by

$$J_{ij}^{+} = (\mathbf{E}_{ij}* + D\mathbf{F}_{ij}*)\,\Phi(x); \quad J_{ij}^{-} = (\mathbf{E}_{ij}* - D\mathbf{F}_{ij}*)\,\Phi(x)$$

assure the continuity of the solution and the normal gradient, if the condition

$$J_{ij}^{-} = J_{ij}^{+} \qquad \text{(IV.13)}$$

(i.e. the entering current at a given face equals the exiting current of the neighboring node and this is true for both sides of the face) is met on the joint boundary ij. On external boundaries, the term on the external side is missing in the above expression, and there Eq. (IV.7) gives the missing term.

Proposition 2. The entering currents can be decomposed by means of (A.2) into irreps. The irreps of the entering current are given by Eq. (II.3), with $g_i(\theta)$ = (constant) = m_i.

Proof: First we prove that **E** and **F** commute with the symmetries of V. A symmetry operation transforms the points of integration into each other, thus, **E** is invariant. The scalar product ∂_n is invariant under the symmetries, thus, a symmetry operation transforms only the range of the integration into another range, and hence F is invariant. Therefore, a symmetry operation of V commutes with **E** and **F**, thus Eq. (A.2) can be applied to project out the irreps of the entering

(exiting) currents $J^+(\theta)$. Thus, the irrep is given by (II.3), but we deal with half-face averaged values. Thus, $g_i(\theta)$ is a constant, say m_i, which completes the proof.

The elementary solutions are exponential functions. When a symmetry operation O is applied to them, the transformation can be transferred from the space variable to the parameter b. When the irreps are formed, the exponential functions with different b parameters are summed with suitable coefficients taken from the character table. Thus, $S_k(b,x)$ will be the k-th irrep, a linear combination of exponentials, with b parameters which are transformed into each other by the symmetries of V. Since there are $2*n_F$ symmetries, the maximal number of terms in the linear combination is $2*n_F$. and there are at most $2*n_F$ independent linear combinations. Thus, a decomposition of the trial function (IV.9) is given by

$$\Phi_j(x) = \sum_{k=1}^{2n_F} c_{jk} S_{jk}(b,x) . \qquad \text{(IV.14)}$$

The condition

$$m_{jk} = c_{jk} \mathbf{E} * S_{jk}(b,x); \quad k = 1,...,2n_F \qquad \text{(IV.15)}$$

determines c_{jk}. These equations are independent, we get each m_{jk} by a single division. At the same time, we have an explicit demonstration of Lemma 4, that the response matrix is diagonal. Since c_{jk} is expressed with m_{jk}, which is the given irrep of the entering current, and the exiting current is given by a matrix multiplied by c_{jk}, see Eq. (IV.14), the elements of the response matrix can be calculated explicitly.

Let us introduce the vectors $\mathbf{J}^+ = (J^+_1, J^+_2,...,J^+_N)$ and $\mathbf{J}^- = (J^-_1, J^-_2,...,J^-_N)$ composed of the partial currents of the nodes in V. Each node has a response matrix $\mathbf{R}_i$. Thus, we get the relationship

$$\mathbf{J}^- = \mathbf{R}\mathbf{J}^+ , \qquad \text{(IV.16)}$$

where $\mathbf{R} = \mathrm{diag}(\mathbf{R}_1,...,\mathbf{R}_N)$. The continuity condition Eq. (IV.13) and the boundary condition on the external boundaries, see Eq. (IV.6), give another relationship between vectors $\mathbf{J}^-$ and $\mathbf{J}^+$:

$$\mathbf{J}^- = \mathbf{G}\mathbf{J}^+ . \qquad \text{(IV.17)}$$

Matrix **G** accounts for the continuity conditions Eq. (V.13) on the internal boundaries and the boundary conditions Eq. (IV.6) on external boundaries. Thus, the structure of matrix **G** depends only on the geometry of V and on the external boundary condition.

Definition 5. The matrix **RG** is called the response matrix (RM) of region V.

Proposition 3. If Φ is the fundamental mode eigenfunction of **A**, i.e. Eq. (IV.9) holds for every j, then the exiting currents are eigenvectors of the matrix **RG** with the largest eigenvalue equal to 1.

Proof: If Φ is a fundamental mode eigenfunction of **A** in V, then in each V_i we get Eq. (IV.5), where the entering currents of the neighboring nodes are taken as given. From Φ, we calculate the exiting currents of V_i. On internal boundaries the fundamental mode solution meets the continuity condition Eq. (IV.13). Thus, we get

$$\mathbf{J}^+ = \mathbf{R}\mathbf{G}\mathbf{J}^+ .$$

Repeating this reasoning n times, we have that for arbitrary n

$$\mathbf{J}^+ = (\mathbf{R}\mathbf{G})^n\mathbf{J}^+ .$$

This implies that the largest eigenvalue of **RG** is one, and the associated eigenvector is $\mathbf{J}^+$ as stated.

Thus, matrix **RG** has a fixed point, and an iteration scheme exists to find that fixed point. The iteration has two levels. At the first level the largest eigenvector of **R**(k)**G** is determined; and at the second, k is set so that the largest eigenvalue of **R**(k)**G** is 1.

The numerical method is flexible with respect to the geometry. All that is required is that the boundary conform to a group of symmetry transformations as is the case in, for example, square, triangular or hexagonal regions in two or three dimensional problems. The method is effective because the problem is broken up into smaller problems; and consequently the gain in large scale problems may be considerable.

2. Application to Neutron Diffusion

The benefit of applying group theory manifests itself in the following simplifications. First of all, a multi dimensional problem becomes one-dimensional in the following sense. All space dependent quantities will have a given pattern of space dependence, especially in diffusion theory. This advantage, recognized long ago, is that we have to deal with the ground only, instead of the full volume. The ground is often small enough to allow for further simplifications, e.g. explicit analytical solution in a hexagonal node. A further simplification is due to the irreps. Instead of solving one big problem, we solve several smaller problems depending on the particular geometry. A matrix multiplication includes N^3 multiplications, if we have 4 irreps (as is the case with a square shaped node), we will have 4 times N^3 multiplications where N is the size of the problem associated with a given irrep. An explicit example will be given later.

The elementary solutions of the diffusion equation (B.1) are given by (B.2), consisting of a vector multiplied by a function. Thus, the irrep formed from the analytical solution will contain cosine, sine and hyperbolic functions depending on the eigenvalue. In a homogeneous region the smallest and largest eigenvalues are real; other eigenvalues may occur in complex conjugate pairs. In the latter case the real part and the imaginary part are treated as separate eigenvectors and eigenvalues. However, it is sufficient to solve the diffusion equation with face averaged fluxes and currents in relatively large nodes.

The first computer program for the solution of the neutron diffusion equation[25] used the following four $\mathbf{e}_i$ vectors in square shaped nodes (c.f. Eq. (II.3)):

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}; \quad \mathbf{e}_2 = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}; \quad \mathbf{e}_3 = \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}; \quad \mathbf{e}_4 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}. \tag{IV.18}$$

The corresponding analytical solutions are

$$\begin{aligned} S_1(x,y) &= \cosh(\lambda_k \mathbf{b}_1 \mathbf{x}) + \cosh(\lambda_k \mathbf{b}_2 \mathbf{x}) \\ S_2(x,y) &= \cosh(\lambda_k \mathbf{b}_1 \mathbf{x}) - \cosh(\lambda_k \mathbf{b}_2 \mathbf{x}) \\ S_3(x,y) &= \sinh(\lambda_k \mathbf{b}_1 \mathbf{x}) * \cosh(\lambda_k \mathbf{b}_2 \mathbf{x}) \\ S_4(x,y) &= \cosh(\lambda_k \mathbf{b}_1 \mathbf{x}) * \sinh(\lambda_k \mathbf{b}_2 \mathbf{x}) \end{aligned} \tag{IV.19}$$

Here b_1 and b_2 are suitable unit vectors, see Ref. [30]. The pattern of the response matrix calculated from the analytic solution is

$$\text{diag}\langle R_1, R_2, R_3, R_4 \rangle \tag{IV.20}$$

where $R_3 = R_4$ because S_3 and S_4 are two components of a two-dimensional irreducible representation. The off-diagonal elements are zero, see (A.5), and according to the Wigner-Eckart theorem, the same diagonal element belongs to different components of a given representation. The R_i matrices depend also on the structure of the diffusion equation through the λ_k eigenvalues and the $\mathbf{t}_k$ eigenvectors (see Eq. (B.3)), either of them bears properties of the energy transfer matrix S in Eq. (B.1). The R_i matrices have the following structure:

$$R_i = (1 - 2\tilde{R}_i)^{-1} (1 + 2\tilde{R}_i), \tag{IV.21}$$

where

$$\tilde{R}_i = -DT\langle G_i(\lambda_k)/F_i(\lambda_k)\rangle T^{-1} \tag{IV.22}$$

with D denoting a matrix composed of the diffusion coefficients, matrix **T** is formed from the eigenvectors $\mathbf{t}_i$ and the part in < > is a diagonal matrix labeled by index k. G_i and F_i in the k-th entry is formed by means of operator **F** and **E**, respectively, from the analytical solution $S_i(x,y)$ with λ_k. In the first hexagonal code (see Ref. [29]), the following vectors have been used:

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}; \quad \mathbf{e}_2 = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}; \quad \mathbf{e}_3 = \begin{pmatrix} 2 \\ -1 \\ -1 \\ 2 \\ -1 \\ -1 \end{pmatrix}; \quad \mathbf{e}_4 = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \end{pmatrix}; \quad \mathbf{e}_5 = \begin{pmatrix} 2 \\ 1 \\ -1 \\ -2 \\ -1 \\ 1 \end{pmatrix}; \quad \mathbf{e}_6 = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ -1 \\ -1 \end{pmatrix}. \tag{IV.23}$$

In the elementary solutions, one b value has been associated with each face (e.g. it may point to mid or corner points). The irreps of the solution are formed as shown by (IV.14). According to theorems A.1 and A.2, the response matrix will take the form

$$\text{diag}\langle R_1, R_2, R_3, R_4, R_4\rangle$$

in hexagonal shaped nodes. The elements of the response matrices are analytical functions of the node size and material properties (i.e. eigenvalues and eigenvectors of matrix S). The structure of the R_i matrices is the same as with the square shaped nodes.

The numerical solution has two major steps. The determination of the largest eigenvalue of **A**(k), and the determination of *k* so that the largest eigenvalue is 1. There are procedures available to solve the first problem, see ARPACK, LAPACK[2] packages. The methods may vary from the simple power method to more sophisticated acceleration methods, see Ref. [20]. In the second problem we simply need a root finding routine. The responses of the nodes are calculated

[2]ARPACK is available at site ftp://ftp.caam.rice.edu/pub/people/kristyn, LAPACK is available at more than 600 web sites including http://netlib.org/lapack/.

from the analytical solutions and the entering currents are decomposed into the $\mathbf{e}_i$ vectors. After calculating the irreps of the exiting currents, the exiting currents on the faces of the node are reconstructed from the irreps. Instead of calculating the spectral ratio, the following physical argument is used. When the new entering currents are known in every node, the new estimated k value is determined from the overall neutron balance. This method, however, has serious limitations. Before passing on to numerical results, let us consider the gain of applying group theory. The first advantage is that using the irreps, we actually deal with four one dimensional problems. The problems are independent. In NG energy groups, to get the exiting currents, we have to perform 36*NG*NG multiplications. Using group theory, we need 4*NG*NG multiplications. As to the determination of the response matrix elements from an analytical solution, we have to invert one matrix of order 6*NG and to multiply it with another matrix. Using group theory, that work reduces to four times (i.e. four irreps) the multiplication of two diagonal matrices **F** and **G** of order NG and two multiplications by **T** and $\mathbf{T}^{-1}$. Additionally, we have to invert one matrix, **T**, of order NG. A further gain is, that having an analytical solution, the iteration may converge faster than with other trial functions.

Below, we investigate the relationship to the two most widely applied methods, finite difference and finite element methods, see Ref. [39]. An analytical solution allows one to start from the analytical solution and to derive the approximations employed in diverse algorithms from that accurate solution. Expression (IV.9) satisfies the DE at each point inside V. Below we show under what conditions that analytical solution leads to the trial functions applied by different methods.

First, the analytical solution (IV.9) allows for a derivation of a modified FD form which is exact in the sense that the same FD equation can be obtained from the following conditions:

- the solution is satisfied at every point in V;
- fluxes and currents are continuous at the node surface in the integral sense;
- the balance equation is formulated only with average fluxes.

The derivation that follows is for hexagonal nodes. The space dependent flux of problem (IV.1) is written as

$$\Phi(r) = \mathbf{T}\left(\langle F_e(r)\rangle \mathbf{c}_e + \langle F_o(r)\rangle \mathbf{c}_o\right), \tag{IV.24}$$

where matrix $\mathbf{T}$ is formed from the eigenvectors t_{ig}. The space dependent part has been decomposed into an even and odd part along with the corresponding constants that have been separated out from the $W_k(B)$ functions. Let us consider the joint boundary of two nodes and the flux averaged over the joint face. The nodes differ in all the three components (viz. $\mathbf{T}$ matrix, c constant and F function), a subscript which will be taken into account by a sunscript. The continuity condition of the face integrated fluxes reads as

$$\mathbf{T}_0\left(\langle \bar{F}_{0e}\rangle \mathbf{c}_{0e} + \langle \bar{F}_{0o}\mathbf{c}_{0o}\rangle\right) = \mathbf{T}_1\left(\langle \bar{F}_{1e}\rangle \mathbf{c}_{1e} + \langle \bar{F}_{1o}\rangle \mathbf{c}_{1o}\right). \tag{IV.25}$$

The boundary flux Φ_b can be given as the average of the boundary fluxes of the two nodes, and the coefficients can be eliminated by means of the fluxes (Φ_i) at the node centers:

$$\Phi_b = \mathbf{T}_0\left(\langle \bar{F}_{0e}\rangle \mathbf{T}_0^{-1}\Phi_0 + \langle \bar{F}_{0o}\rangle \mathbf{c}_{0o}\right) = \mathbf{T}_1\left(\langle \bar{F}_{1e}\rangle \mathbf{T}_1^{-1}\Phi_1 + \langle \bar{F}_{1o}\rangle \mathbf{c}_{1o}\right). \tag{IV.26}$$

Similarly, the continuity of the normal current is assured by

$$-\langle D_0\rangle \mathbf{T}_0\left(\langle G_{0e}\rangle \mathbf{T}_0^{-1}\Phi_0 + \langle G_{0o}\rangle \mathbf{c}_{0o}\right) = \langle D_1\rangle \mathbf{T}_1\left(\langle G_{1e}\rangle \mathbf{T}_1^{-1}\Phi_1 + \langle G_{1o}\rangle \mathbf{c}_{1o}\right). \tag{IV.27}$$

Thus, the boundary current is a linear expression of the fluxes at the node centers.

Introducing the following matrices

$$\begin{aligned}
\rho_0^e &= T_0\langle F_{0e}\rangle T_0^{-1};\ \delta_0 = \langle D_0\rangle T_0\langle G_{0e}\rangle T_0^{-1} \\
\rho_1^e &= T_1\langle F_{1e}\rangle T_1^{-1};\ \delta_1 = \langle D\rangle T_1\langle G_{1e}\rangle T_1^{-1} \\
f_0 &= T_0\langle F_{0o}\rangle;\ d_0 = \langle D_0\rangle T_0\langle G_{0o}\rangle \\
f_1 &= T_1\langle F_{1o};\ d_1 = \langle D_1\rangle T_1\langle G_{1o}\rangle
\end{aligned} \quad , \tag{IV.28}$$

we obtain the boundary flux and current

$$\Phi_b = \left[\mathbf{d}_0\mathbf{f}_0^{-1} + \mathbf{d}_1\mathbf{f}_1^{-1}\right]^{-1}\left[\delta_0\Phi_0 + \delta_1\Phi_1\right] \tag{IV.29}$$

$$\mathbf{J}_b = \left[\mathbf{f}_0\mathbf{d}_0^{-1} + \mathbf{f}_1\mathbf{d}_1^{-1}\right]^{-1}\left[\left(\mathbf{f}_0\mathbf{d}_0^{-1} - \rho_0^e\Phi_0\right) - \left(\mathbf{f}_1\mathbf{d}_1^{-1} - \rho_1^e\Phi_1\right)\right] . \tag{IV.30}$$

In Eqs. (IV.26), the space dependent part of the solution has been integrated over a face, in (IV.27) the normal gradient has also been integrated over a face; these transformations are in <>. The two latter equations allow us to express the boundary fluxes and currents as linear expressions of the flux at the respective node centers. For the balance equation we need an expression for the volume integrated flux. This is achieved by integrating the analytical formula for the flux over one sixth of the node, i.e. over a regular triangle, to arrive at

$$\bar{\Phi}_{01} = \mathbf{v}_0\Phi_0 + \mathbf{w}_0\left[\left[\mathbf{d}_0\mathbf{f}_0^{-1} + \mathbf{d}_1\mathbf{f}_1^{-1}\right]^{-1}\left[\delta_0\Phi_0 + \delta_1\Phi_1\right] - \rho_0^e\Phi_0\right] . \tag{IV.31}$$

The expressions for the other five triangles are similarly obtained. (Matrices $\mathbf{v}_0$ and $\mathbf{w}_0$ denote integrals of $\langle F_{0e}\rangle$ and $\langle F_{0o}\rangle$ over one sixth of the hexagon.)

In order to get the traditional FD scheme, we retain only the fundamental buckling in expression (IV.14), and assume that

$$\lambda r \ll 1 \ ,$$

and the constant and linear terms approximate well the exponential in (IV.9). One then arrives at the following expressions for the boundary flux and current:

$$\mathbf{\Phi}_b = \frac{2}{H}\left[\langle D_1\rangle + \langle D_0\rangle\right]^{-1}\left[\langle D_1\rangle\mathbf{\Phi}_1(0) + \langle D_0\rangle\mathbf{\Phi}_0(0)\right], \tag{IV.32}$$

$$\mathbf{J}_b = -\frac{2\langle D_0\rangle}{H}\left[\mathbf{\Phi}_b - \mathbf{\Phi}_0(0)\right] \tag{IV.33}$$

which are the fundamental expressions of the finite difference equations. (The bold flux and current represent vectors formed from the energy group fluxes and currents. Diagonal matrices are denoted by <>. Subscript b refers to the boundary.) Thus, the flux at the node center equals the average flux.

The desire to extend the FD formalism beyond the small mesh limit is justified. Introducing a matrix coefficient set, which couples the different energy groups, can achieve that goal and both the boundary flux and the current can be expressed as linear functions of the fluxes at the node centers, whatever the mesh size, whatever the material properties of the nodes.

In order to get the FE method expression for the flux, let us retain the first few low order terms in the space dependent part of expression (IV.9):

$$\begin{aligned}\Phi_g &= \sum_{k=1}^{G} t_{kg} \sum_{n=0}^{N} r^n \int_{|B|=1} W_k(B)(\lambda_k B)^n dB + R_N \\ &= \sum_{n=0}^{N} c_{gn} r^n + R_N \,.\end{aligned} \tag{IV.34}$$

The remainder R_N tends to zero in Eq.(IV.34) as N tends to infinity. This approximation is reasonable, if the expansion is confined to a finite small volume and the cross-sections are such that the constraint $\lambda_k r<1$ holds for every k. In most reactor models, this is true only for the fundamental

eigenvalue but not for the transients. Consequently, the approximation is better for volume averages than for pointwise quantities. This approximation is called nodal expansion method (NEM). Usually the unknown c_{gn} coefficients are expressed by face or volume averaged fluxes or currents. The coarse mesh finite difference (CMFD) method stops at *n=0*; the flux is considered as constant in a node. The current is eliminated from the integral balance with the help of the FD formalism presented above. When the unknown coefficients c_{gn} are expressed by pointwise fluxes in every node, we get the FE method.

The proposed method can be formulated as a variational problem. We look for the minimum of the linear functional

$$\mathcal{L} = \left(\Psi(x);\ A\Phi(x)\right)_V \tag{IV.35}$$

where $\Psi(x)$ is an arbitrary function. Substituting the diffusion operator for **A**, and using the Green's formula, we get the following expression:

$$\mathcal{L} = \left(\mathbf{A}^{+}\Psi(x);\ \Phi(x)\right)_V + \left(\partial_n\Psi(x);\ \Phi(x)\right)_{\partial V} + \left(\Psi(x);\partial_n\Phi(x)\right)_{\partial V}. \tag{IV.36}$$

For a minimum, each term in the above equation must vanish. The volume integral vanishes when $\Psi(x)$ is the adjoint function. The surface integral can be expanded into two terms, and when (IV.2) is introduced into (IV.35), the surface integral $\mathcal{L}$ reduces into internal ($\Delta\mathcal{L}_i$) and external ($\Delta\mathcal{L}_e$) surface integrals $\mathcal{L} = \Delta\mathcal{L}_i + \Delta\mathcal{L}_e$:

$$\Delta\mathcal{L}_i = \sum_{j=1}^{N} \int_{\partial V_j} \Psi(x)\left(\partial_{n_j}\Phi_j(x) - \partial_{n_j'}\Phi_j'(x)\right)dF + \int_{\partial V_j} \partial\Psi_n(x)\left(\Phi_j(x) - \Phi_j'(x)\right)dF \tag{IV.37}$$

$$\Delta\mathcal{L}_e = \sum_{j=1}^{N} \int_{\partial V} \Psi(x)\left(\partial_n\Phi_j(x)\right)dF + \int_{\partial V} \partial\Psi_n(x)\left(\Phi_j(x)\right)dF. \tag{IV.38}$$

In Eq. (IV.37), we excluded those faces of ∂V_j which are external surfaces; only those nodes contribute to integral (IV.38) which have at least one face on the external surface ∂V. Now the solution is expanded in terms of a set of orthogonal basis functions as follows. Let

$$\Phi(x) = \sum_{j=1}^{N} \sum_{k=1}^{n_F} c_{jk}\varphi_{jk}(x) \ . \qquad \text{(IV.39)}$$

The basis functions possess the following properties: for all k, $\varphi_{jk}(x)=0$ if $x \in V\text{-}V_j$ whereas in V_j they obey Eq. (IV.5). Furthermore, $\varphi_{jk}(x)$ transforms as the k-th irreducible component of the solution to the DE in volume V_j. The basis functions are orthogonal by Theorem A.2. In order to find the c_{jk} coefficients, we require either component of $\mathcal{L}$ to be zero when the weight functions are $\mathbf{e}_{k'}$ see Section II, in each surface integral. Because of the basic Lemma, the solution in V_j transforms according to the k-th irrep, if the boundary condition is proportional to $\mathbf{e}_k$. Selecting the weight function Ψ_{jk} proportional to $\mathbf{e}_k$ in volume V_j and zero elsewhere in V, and making use of Theorem A.4 we get a set of equations for c_{ik}. :

$$\left\langle \Psi_{j'k'}; \mathbf{A}\varphi_{jk} \right\rangle_V = \delta_{j'j}\delta_{k'k} \left[\left\langle c_{jk}\partial\varphi_{jk} - c_{j'k'}\partial\varphi_{j'k'} \right\rangle_{\partial V_j} + \left\langle c_{jk}\varphi_{jk} - c_{j'k'}\varphi_{j'k'} \right\rangle_{\partial V_j} \right]. \qquad \text{(IV.40)}$$

This set is solved recursively in Section VI under the hypotheses that the diffusion operator is completely continuous and the iteration converges from any initial vector not orthogonal to the solution.

Various numerical benchmark problems have been investigated and compared to the standard methods. We present two cases for square and hexagonal geometry. In square geometry, volume V involved 28 squares of 20 cm x 20 cm. The order of the eigenvalue error is $\sim 10^{-4}$, see Ref. [28]. In hexagonal geometry, abundant experience has been collected for light water reactors. There the distance between the centers of two hexagons is 14.7 cm and 23.4 cm, see Ref. [32], the error of the eigenvalue is in the order of 10^{-4}. A short intercomparison is given from Ref. [30]. The test case presented is GA9A1, (see Ref. [1]), which models a high temperature gas cooled rector

core, in hexagonal geometry; the distance between the centers of neighboring hexagons is h = 36.2 cm. The codes in the comparison are well known production codes. The reference eigenvalue is $k_{eff} = 1.1183 \pm 0.0001$, obtained by extrapolation. Table II compares the eigenvalues and the error in the power distribution (ΔP, in percent), (see Appendix B). The code HEXAN incorporates the above presented group theoretic considerations. If a date is not available, star (*) is used in Table II.

Table II. Comparison of GA9A1 Test Results

(*-datum not available)

Program	k_{eff}	Points/Node	ΔP
BUG 180	1.11815	48	0
GRIMHX	1.11863	6	3.1
VENTURE	1.1186	54	*
VALE	1.11596	3	3.3
DIFGEN	1.117	38	4.7
M2	1.11824	1	*
HEXAN	1.11888	1	2.2
Reference	1.1183	*	*

At present there exist several multigroup diffusion theory codes in two or three dimensions [3, 4, 17, 32] which include to various degrees the above group theoretical principles. These codes are routinely applied in nuclear reactor design and operation to problems which require up to 3490 nodes, and two to four energy groups at each node. The maximal error in the nodewise average flux is 2-4%, the error of the eigenvalue is in the order of 10^{-4}.

Results of a three dimensional benchmark with hexagonal nodes is presented in Fig. 4. The distance between the centers of two hexagons is 14.7 cm. The height of the hexagons is 25 cm, the lower part has one composition and the upper part is different due to the control rods in positions 1 and 7. Each hexagon is subdivided into 10 axial layers, 25 cm each. The sum of the powers of the 10 layers are shown in Fig. 4. The reference solution was derived by finite difference version[24] of the code DIF3D, by means of extrapolation. The finest mesh was 1.4145 cm triangular, and 2.5 cm axial. The maximum deviation between the DIF3D solution solution and the extrapolated solution was 0.66%. In Fig. 4 the upper number is a numbering of the hexagons, the middle number is the relative power density calculated by HEXAN, the lower number is the difference in percent between the HEXAN power density and the extrapolated FD solution. The error in Fig. 4 increases towards the external boundary (assembly Nos. 59, 55, 56, 52, 47, 41, 27, and 19) because of the poor representation of the boundary. The maximum error is 1.2%. HEXAN used only one entering current value per face per energy group.

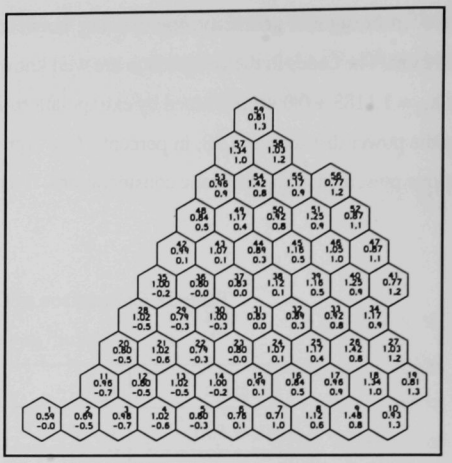

Fig. 4. SEIDEL Benchmark Results

V. PROBLEM SIZE REDUCTION

In Section IV, the solution of a boundary value problem was reduced to an algebraic problem with one unknown per face, by an approximation based on symmetry projections of an elementary solution. It will now be shown that the size of the algebraic problem can be reduced further, and one unknown per subvolume is sufficient, if only the continuity of face averages is required. In the second part, we deal with the application of group theory to non-symmetric operators, i.e. when operator A may have no symmetry at all.

1. Elimination of Asymmetric Components

Although the finite difference method is bound to fine meshes, an indisputable benefit of the method is its simplification; only one unknown per node is involved. Following an earlier work,[32] it will be shown that we are able to reduce the size of the problem with the help of the continuity conditions of the solution and its gradient. The irreps turn out to satisfy an equation which is an extension of the finite-difference formula; and after eliminating the non-symmetric terms, an equation is obtained for the symmetric component (unit representation). It is known that this is the only representation contributing to node averaged solution.

Thus, we obtain an equation for node averages by writing the entering currents at the four faces of node j into the following form:

$$\begin{pmatrix} I_{j1} \\ I_{j2} \\ I_{j3} \\ I_{j4} \end{pmatrix} = X_{j1} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} + X_{j2} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} + X_{j3} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} + X_{j4} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} \tag{V.1}$$

where

$$X_{j1} = (I_{j1} + I_{j2} + I_{j3} + I_{j4})/4 \tag{V.2a}$$

$$X_{j2} = (I_{j1} - I_{j3})/2 \tag{V.2b}$$

$$X_{j3} = (I_{j2} - I_{j4})/2 \tag{V.2c}$$

$$X_{j4} = (I_{j1} - I_{j2} + I_{j3} - I_{j4})/4 \ . \tag{V.2d}$$

Note that the vectors utilized in Eq.(V.1) are just the simplified irreps shown in Fig.2 and denoted by $\mathbf{e}_i$, c.f. Eq.(II.3). The following node numbering notation is specified for the continuity condition (IV.13). The node with subscript j = 0 is surrounded by nodes j = 1, j = 2, j = 3, and j = 4 in such

a way that node i attaches to node j = 0 at side i, see Figure 5. With the help of the response matrix (IV.16), the exiting currents of a given node are expressed as

$$\mathbf{I}_j^+ = R_{j1}X_{j1}\mathbf{e_1} + R_{j2}X_{j2}\mathbf{e_2} + R_{j3}X_{j3}\mathbf{e_3} + R_{j4}X_{j4}\mathbf{e_4} . \tag{V.3}$$

After rearranging the terms, $R_{j4} = R_{j3}$ and the continuity condition (IV.13), give a set of equations for the irreps X_{j1}, X_{j2}, X_{j3} and X_{j4}, j = 1,...,N as follows:

$$\frac{1}{4}\sum_{j'=1}^{4}\left(X_{01} - \mathbf{R}_{j'1}X_{j'1}\right) = Q_{01} . \tag{V.4}$$

where the source term Q_{01} is given as

$$\begin{aligned} Q_{01} = {} & \boldsymbol{R}_{32}X_{32} - \boldsymbol{R}_{12}X_{12} + \boldsymbol{R}_{43}X_{43} - \boldsymbol{R}_{23}X_{23} + \boldsymbol{R}_{14}X_{14} - \boldsymbol{R}_{24}X_{24} \\ & + \boldsymbol{R}_{24}X_{24} + \boldsymbol{R}_{34}X_{34} - \boldsymbol{R}_{44}X_{44} \end{aligned} \tag{V.5}$$

Other irreps satisfy similar equations of the form

$$\frac{1}{k_i}\sum_{j'=1}^{4}\left(X_{0i} - r_{j'}X_{j'i}\right) = Q_{0i} , \tag{V.6}$$

where k_i is a constant. The $r_{j'}$ coefficients are composed of the response matrices and the source is independent of X_{i0}. The above expressions are slightly modified forms of the finite- difference equations. The first equation, (V.4) is exactly the finite-difference equation. Thus, the set of the continuity equations has been reformulated as a set of coupled, modified finite-difference equations. The structure of the equations is as follows:

$$\mathbf{X}_i = \sum_{j=1}^{4}\mathbf{M}_{ij}\mathbf{X}_j , \tag{V.7}$$

and using the following partitioning $x = X_1$; $y = (X_2, X_3, X_4)$, we can eliminate y:

$$\begin{pmatrix} M_{xx} & M_{xy} \\ M_{yx} & M_{yy} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} \tag{V.8}$$

$$y = \left(1 - M_{yy}\right)^{-1} M_{yx} x \tag{V.9}$$

$$\left(M_{xx} + M_{xy}\left(1 - M_{yy}\right)^{-1} M_{yx}\right) x = x \tag{V.10}$$

The only condition is the invertibility of $(1\text{-}M_{yy})$. To show that M_{yy} is invertible, it is sufficient to show that the rows and columns of the lower matrix are independent. M_{yy} is a three by three block in Eq.(V.7), which we rewrite as

$$\mathbf{M} = \begin{pmatrix} F_2 & q_{23} & q_{24} \\ q_{32} & F_3 & q_{34} \\ q_{42} & q_{43} & F_4 \end{pmatrix}$$

where F_i is the modified FD matrix associated with X_i, and q_{ij} is the source term representing the contribution of u_j in the equation for X_i. Every F_i is invertible because the modified FD problem has a solution with a source, q_{ij} differs from F_i for all i and j. Thus, both the rows and the columns are linearly independent.

After the above reduction, we get a set of equations with one unknown per node. When we deal with the diffusion equation, the unknown is the node average flux, the average value of the solution. This is because the integral balance gives an immediate relationship between u_1 and the average flux. That reduction means that the number of unknowns reduces by a factor of four (in square nodes) or six (in hexagonal nodes) without introducing any approximation.

2. Non-Symmetric **A** Operator

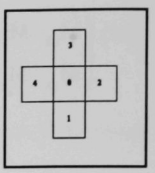

Fig. 5. Node Numbering

Let us consider the BVP (II.2). In the previous sections, the investigations have been limited to cases when there is a group which leaves the problem invariant. As we saw in Section II, given an arbitrary group, the solution space can be split into orthogonal subspaces. Furthermore, if the elements of the group commute with the BVP, the subspaces remain separated during the iteration because any operator utilized in the iteration will be diagonal.

In this section, the investigation is extended to cases where the elements of the group do not commute with the operators in the problem. It will be shown, that the iteration can be transformed to a form where subspaces $S^{(\alpha)}$ of the solution space S remain linearly independent during the solution. Thus, any group induces a splitting of the solution space into independent subspaces.

The problem is discussed in the following formulation. The iteration is summarized as the numerical solution of the problem

$$\mathbf{A}\Phi = a\Phi \,, \tag{V.11}$$

where **A** is a matrix, and $\Phi \in S$ is the solution to be determined. Let a G group be given, e.g. the group transforming the region V into itself. We assume **A** not to commute with the elements of G. Then, **A** can be decomposed into irreps the same way as a function is decomposed, see Ref. [25], Section 6.1. Let the decomposition of **A** and of Φ be

$$\mathbf{A} = \sum_k \sum_\alpha \mathbf{A}_k^{(\alpha)} \tag{V.12}$$

$$\Phi = \sum_k \sum_\alpha c_k^{(\alpha)} \Phi_k^{(\alpha)} \,. \tag{V.13}$$

Superscript (α) refers to the invariant subspace, k assigns the basis in the subspace. In order to simplify the notation, the irreps are renumbered from 1 to h. The eigenvalue problem (V.11) is written as

$$\sum_i (\mathbf{A}_i) \sum_j (c_j \Phi_j) = a \sum_k c_k \Phi_k \,. \tag{V.14}$$

Let us multiply this expression by Φ_p:

$$\sum_{i,j} (\Phi_p; \mathbf{A}_i \Phi_j) = a c_p \tag{V.15}$$

because of the orthogonality of the basis vectors. According to the Wigner-Eckart theorem, see Appendix A, the product $\mathbf{A}_i\Phi_j$ is a direct product that can be decomposed into irreps with the help of the Clebsch-Gordan coefficients (in short CGC) $C_{k,ij}$ and we arrive at

$$\sum_{i,j} (\Phi_p; C_{p,ij} \Phi_p) c_j = a c_p \tag{V.16}$$

where

$$\mathbf{A}_i \Phi_j = \sum_k C_{k,ij} \Phi_k \quad . \tag{V.17}$$

The p-th component of the solution vector contains only contribution from those $\mathbf{A}_i\Phi_j$ products, for which the CGC is non-zero. In other words, Eq. (V.17) has the following structure:

$$\sum_j \mathbf{U}_{ij} \Phi_j = a \Phi_j \tag{V.18}$$

where the elements of the block matrix $\mathbf{U}_{ij}$ is composed of the $\mathbf{A}_1,...,\mathbf{A}_h$ components of $\mathbf{A}$. Furthermore, the matrix $\mathbf{U}_{ij}$ is symmetric because the CGCs are symmetric. Let $\mathbf{P}$ transform $\mathbf{U}_{ij}$ into a lower triangular matrix L:

$$\mathbf{L} = \mathbf{PUP}^{-1} ,$$

then, it suffices to determine the first element of $\mathbf{P\Phi}$ in order to find the solution of Eq. (V.11). Indeed, let us multiply (V.11) by $\mathbf{P}$ from the front and use the identity $\Phi = \mathbf{P}^{-1}\mathbf{P\Phi}$. Because $\mathbf{PUP}^{-1}$ is lower triangular, the first equation reads as

$$L_{11}(P\Phi)_1 = a(P\Phi)_1 .$$

This is an eigenvalue problem in a subspace of S. If that eigenvalue is solved, the other elements of $\mathbf{P\Phi}$ can be determined by the forward elimination, backward substitution method.

Proposition 4. Let $\mathbf{A}$ be a given linear operator, G a given group of h elements mapping S into itself. Then the iteration

$$\mathbf{A}\Phi_k = a_k\Phi_{k+1}; \quad \Phi_k \in S \text{ for } k = 1,2,...$$

can be reduced to the subspace $(\mathbf{P\Phi})_1$, where $\mathbf{P}$ is a matrix which transforms $\mathbf{U}_{ij}$, into a lower triangular form. Here Φ is the vector of invariant components (induced by G) of the solution, the $\mathbf{U}_{ij}$ matrix is formed by the CGC according to (V.17).

Let us consider the C_i group as a particular case with external source. Let the equation be the diffusion equation

$$\left(\frac{d^2}{dx^2} + f(x)\right)\Phi(x) = q(x)$$

where f(x) is given. Let the solution space S be the functions of twice differentiable functions in the interval V. The solution is decomposed into even (Φ_e) and odd (Φ_o) components. The operator is also decomposed into even (A_e) and odd (A_o) parts. The CGCs give the even and odd combinations:

$$\begin{pmatrix} A_e & A_o \\ A_o & A_e \end{pmatrix} \begin{pmatrix} \Phi_e \\ \Phi_o \end{pmatrix} = \begin{pmatrix} q_e \\ q_o \end{pmatrix}$$

which is transformed into lower diagonal form by

$$P = \begin{pmatrix} A_o^{-1} & -A_e^{-1} \\ A_e^{-1} & A_o^{-1} \end{pmatrix},$$

and we have to solve

$$\left(A_o^{-1}A_e - A_e^{-1}A_0\right)\Phi_e = \left(A_o^{-1}q_e - A_e^{-1}q_o\right)$$

and

$$2\Phi_e + \left(A_e^{-1}A_o + A_o^{-1}A_e\right)\Phi_o = \left(A_e^{-1}q_e + A_o^{-1}q_o\right).$$

The first equation is in the even subspace, the second one in the odd subspace. It suffices to solve the first problem, and substitute Φ_e into the second problem. Hence, even if the operator does not commute with the group, the problem can be reduced.

If the investigated volume is subdivided into nodes and the connection between the node is taken into account by prescribing the continuity of certain quantities, c.f. (IV.13), the above derivation is meaningful only if the continuity equations can also be reduced. In Section IV.1, we showed how to derive finite-difference like equations from the continuity conditions. Using similar arguments, we show how to eliminate the non-symmetric components from the continuity equations

retaining only the unit representation, or, what is equivalent to it, the node averaged value of the solution.

Put the continuity conditions into a linear equation as

$$\sum_{i,j} G_{ij} J_{ij}^{+} = 0 \qquad \text{(V.19)}$$

here subscript i and j refers to the node number and to the face, respectively. The geometry matrix **G** has 0 and a combination of RM elements as entries, see Eq. (IV.17). The J^{+} values on the boundary are transformed into irreps as

$$J_{ij}^{+} = \sum_{k} \omega_{jk} u_{ik} \ , \qquad \text{(V.20)}$$

where ω is an orthogonal matrix. Introducing new variables as

$$H_{ik} = \sum_{j} G_{ij} \omega_{jk}$$

and

$$\mathbf{v_k} = \left(u_{1k},\ldots,u_{Nk}\right)$$

we arrive at the following expression:

$$\begin{pmatrix} C_{11} & C_{12} & \ldots C_{1n_F} \\ \ldots & & \\ C_{n_F 1} & C_{n_F 2} & C_{n_F n_F} \end{pmatrix} \begin{pmatrix} \mathbf{v_1} \\ \ldots \\ \mathbf{v_{n_F}} \end{pmatrix} = 0 \, . \qquad \text{(V.21)}$$

The rank of the matrix in this equation is the same as the rank of matrix **G** because every utilized transformation is invertible. The rank of matrix **G** is $n_F * N_{node}$ -1 because if any element of J^{+} is given, Eq. (V.19) has a unique solution. The elements of the first row are not zero thus every

component is expressible with $\mathbf{v}_1$. Hence, the continuity equations can be reduced to the symmetric component, which in turn is proportional to the node average.

VI. ARBITRARILY ACCURATE COARSE-MESH SOLUTION TO NEUTRON DIFFUSION

The present Section is devoted to an application of the results of Section IV. to the neutron diffusion equation. We assume volume V consists of square sub volumes (nodes), and the number of neutron energy groups is two.

The notion is that the trial functions (IV.8), with several b values satisfy the diffusion equation inside each V_i. Then, if the trial functions can be made to match a boundary value close to the exact solution's boundary value, expression (IV.9) results in an arbitrarily accurate solution. Let $\varphi(\xi)$ be a function that gives the exact boundary value. Let us expand φ into a Fourier series, then it is clear we have to retain those b values which are present in the Fourier spectrum of φ. It is known that the entering current distribution on the boundary is adequately represented by low order (up to second order) polynomials.[48] If the values $(b_1,...,b_k)$ are chosen so that the first k moments of the trial function take given values, the error inside V_i will depend on the residual term. Let the $\varphi(\xi)$ be sufficiently smooth then we can decompose the function into a polynomial part and a residual as

$$\varphi(\xi) = \sum_{k=1}^{n} c_k \xi^k + \epsilon_n(\xi) \ .$$

Then, an upper error bound of the trial function will be

$$\delta\Phi_n(\xi) = \epsilon_n(\xi) * E(\xi)$$

where $E(\xi)$ is the solution to the diffusion equation with the condition that the solution is unity at every boundary point. $E(\xi)$ is a bounded function, $\epsilon_n(\xi)$ tends to zero as n increases (see Weierstrass

approximation theorem in Ref. [39] p. 28). Thus, in principle arbitrary accuracy can be achieved in V_i.

It follows from the discussion of the variational principle in Section IV, that we may find the amplitudes of the irreps in each cell recursively so that the entering current (or the flux) is given by the irrep of the neighbors taken from the previous iteration. It is reasonable to iterate for c_{ik}, $k = 1,...,n_F$ in one step, instead of repeating the iteration n_F times. This can be achieved by taking proper account of the boundary condition. In node j, we collect the entering current and decompose it into irreps. Then the irreps are treated separately and after the last irrep the exiting currents are reconstructed on the faces. Thus, the calculation consists of the following steps, see Refs. [31, 33].

(1) Starting from a positive initial guess, we determine moments of the entering currents on the boundary. Each moment is decomposed into irreps by the projector (A.6). The result is as given in Section II, $\xi^n \mathbf{e}_k$, where ξ is in [-H,+H]. Let the irreps of the zero-th moment be (I_1, I_2, I_3, I_4), the first moments (J_1, J_2, J_3, J_4), the second moments (K_1, K_2, K_3, K_4). The irreps will be as given in Table III. (We recall that the index determines the values at the four faces, e.g. I_1, J_1 and K_1 is proportional to vector $\mathbf{e}_1$, see Eq.(II.3).)

Table III. Irreps of At Most Second Moments

Irrep	Analytical Solution	Vectors
A_1	cosh(a*x)cosh(b*y) + cosh(a*y)*cosh(b*x)	(I_1, K_1)
A_2	sinh(b*x)*sinh(a*y) - sinh(a*x)*sinh(b*y)	(I_2, K_2)
B_1	cosh(a*x)cosh(b*y) - cosh(a*y)*cosh(b*x)	(J_1)
B_2	sinh(b*x)*sinh(a*y) - sinh(a*x)*sinh(b*y)	(J_2)
E_1	cosh(a*x)*sinh(b*y)	(I_3, J_4, K_3)
E_2	cosh(a*y)*sinh(b*x)	(I_4, J_3, K_4)

(2) The corresponding analytical solutions shown in Table III., have also been derived by (A.6), where the response matrix was calculated as in (IV.21) and (IV.22). It should be noted that the different moments mix in some representations. For example, when using second order polynomials, we have the following basis in the six classes of the square: (I_1,K_1), (I_2,K_2), J_1, J_2, (I_3,J_4,J_3), (I_4,J_3,K_4). Here I_k, J_k and K_k are the amplitudes of the zero-th, first and second moments, respectively, each proportional to $\mathbf{e}_k$. The first two vectors belong to the unit representation, and so on. Altogether, we have two two-dimensional, two one-dimensional and two three-dimensional representations. The final form of the response matrices is given below. In the first irrep, we have two vectors and the RM is:

$$\begin{pmatrix} I_1^+ \\ K_1^+ \end{pmatrix} = \mathbf{T}\begin{pmatrix} \mathcal{F}_0 f_{11} & \mathcal{F}_0 f_{21} \\ \mathcal{F}_2 f_{11} & \mathcal{F}_2 f_{21} \end{pmatrix}\begin{pmatrix} \mathcal{E}_0 f_{11} & \mathcal{E}_0 f_{21} \\ \mathcal{E}_2 f_{11} & \mathcal{E}_2 f_{21} \end{pmatrix}^{-1} * \mathbf{T}^{-1}\begin{pmatrix} I_1^- \\ K_1^- \end{pmatrix} .$$

The second representation is again two dimensional:

$$\begin{pmatrix} I_2^+ \\ K_2^+ \end{pmatrix} = \mathbf{T}\begin{pmatrix} \mathcal{F}_0 f_{12} & \mathcal{F}_0 f_{22} \\ \mathcal{F}_2 f_{12} & \mathcal{F}_2 f_{22} \end{pmatrix}\begin{pmatrix} \mathcal{E}_0 f_{12} & \mathcal{E}_0 f_{22} \\ \mathcal{E}_2 f_{12} & \mathcal{E}_2 f_{22} \end{pmatrix}^{-1} * \mathbf{T}^{-1}\begin{pmatrix} I_2^- \\ K_2^- \end{pmatrix} ,$$

whereas the third representation is one dimensional:

$$J_2^+ = \mathbf{T}[\mathcal{F}_1 f_{14}] * [\mathcal{E}_1 f_{14}]^{-1}\mathbf{T}^{-1} J_2^- .$$

The fourth representation is again one dimensional:

$$J_1^+ = \mathbf{T}[\mathcal{F}_1 f_{13}] * [\mathcal{E}_1 f_{13}]^{-1}\mathbf{T}^{-1} J_1^- .$$

The fifth representation is three dimensional:

$$\begin{pmatrix} I_3^+ \\ J_4^+ \\ K_3^+ \end{pmatrix} = \mathbf{T} \begin{pmatrix} \mathcal{F}_0 f_{16} & \mathcal{F}_0 f_{26} & \mathcal{F}_0 f_{36} \\ \mathcal{F}_1 f_{16} & \mathcal{F}_1 f_{26} & \mathcal{F}_1 f_{36} \\ \mathcal{F}_2 f_{16} & \mathcal{F}_2 f_{26} & \mathcal{F}_2 f_{36} \end{pmatrix} \begin{pmatrix} \mathcal{E}_0 f_{16} & \mathcal{E}_0 f_{26} & \mathcal{E}_0 f_{36} \\ \mathcal{E}_1 f_{16} & \mathcal{E}_1 f_{26} & \mathcal{E}_1 f_{36} \\ \mathcal{E}_2 f_{16} & \mathcal{E}_2 f_{26} & \mathcal{E}_2 f_{36} \end{pmatrix}^{-1} * \mathbf{T}^{-1} \begin{pmatrix} I_3^- \\ J_4^- \\ K_3^- \end{pmatrix},$$

and the sixth representation is also three dimensional:

$$\begin{pmatrix} I_4^+ \\ J_3^+ \\ K_4^+ \end{pmatrix} = \mathbf{T} \begin{pmatrix} \mathcal{F}_0 f_{15} & \mathcal{F}_0 f_{25} & \mathcal{F}_0 f_{35} \\ \mathcal{F}_1 f_{15} & \mathcal{F}_1 f_{25} & \mathcal{F}_1 f_{35} \\ \mathcal{F}_2 f_{15} & \mathcal{F}_2 f_{25} & \mathcal{F}_2 f_{35} \end{pmatrix} \begin{pmatrix} \mathcal{E}_0 f_{15} & \mathcal{E}_0 f_{25} & \mathcal{E}_0 f_{35} \\ \mathcal{E}_1 f_{15} & \mathcal{E}_1 f_{25} & \mathcal{E}_1 f_{35} \\ \mathcal{E}_2 f_{15} & \mathcal{E}_2 f_{25} & \mathcal{E}_2 f_{35} \end{pmatrix}^{-1} * \mathbf{T}^{-1} \begin{pmatrix} I_4^- \\ J_3^- \\ K_4^- \end{pmatrix}.$$

In the above expressions, the following notation has been employed. Operators $\mathcal{E}_i$ and $\mathcal{F}_i$ form the i-th moment of the entering and exiting current. The second subscript of the functions f refers to the irrep; the first subscript to the buckling vector b. The continuity of the partial current is assured in one iteration step by taking the exiting currents of the neighboring nodes from the previous iteration. They are decomposed into irreps, the exiting currents of the actual node are determined and then we pass on to the next node. One iterational step includes a sweep through all nodes.

(3) Making use of Lemma 1 in Section IV, the dominant eigenvector is determined. This will be the exiting current vector at the internal and external surfaces.

(4) By means of Lemma 1, we iterate on the free parameter in the neutron cross-sections (c. f. (B.4)) to set the dominant eigenvalue 1. In the iteration the $\alpha(k)$ function is locally approximated by a second order polynomial.

(5) When the iteration has converged, the flux is determined from the analytical solution.

Such a procedure can be expanded to include higher moments. The more moments are retained, the more buckling vectors need to be used and the response matrix becomes correspondingly larger. Thus, the number of retained moments depends on the required accuracy.

To illustrate the capability of the method, we give the results of a simple test problem. The solution of the two energy group diffusion equation is sought in a square which consists of one material with the two energy groups neutron cross-sections given below.

$$D_1 = 1.5 \;\; D_2 = 0.4, \; \Sigma_{a1} = 0.01 \;\; \Sigma_{a2} = 0.08 \;\; \Sigma_{12} = 0.02 \;\; \nu\Sigma_{f1} = 0 \;\; \nu\Sigma_{f2} = 0.135.$$

The region is a square, with sides of 100 units in length, and the boundary condition is $\Phi = 0$. The solution to this problem is $\Phi(x,y) = \cos(x*\pi/100)*\cos(y*\pi/100)$ and $k_{eff} = 1.01397$. The eigenvalue obtained by the algorithm given above is $k_{eff} = 1.01375$, the error of the spatial distribution is less then 10^{-4}, whereas the ratio of the energy group 2 to energy group 1 flux indicates an error of 0.5%. In the calculation the buckling vectors B_1 = (0.51, 0.7399), B_2 = (9.875, i*9.824237), B_3 = (1.0033,0.0813074) have been utilized. The results are rather sensitive to the selection of the B vectors.

VII. CONCLUSIONS

The present work demonstrated the application of group theory to boundary value problems. In Section 2, we formulated three important statements. The first, asserts the smoothness of the irreps, i.e. if the boundary condition is n times differentiable, so are its irreps. This statement assures that a numerical procedure based on irreps will not result in a less smooth solution than the true solution. The second statement, the Basic Lemma, asserts that the solution belongs to the same irrep as the boundary condition. The third statement expresses a feature of the boundary condition, that is, the irreps of the boundary condition can always be expressed by step functions, see Lemma 2. Although Lemma 2 is a straightforward consequence of Theorem A.2., it has a rather important implication in physics. Namely, any boundary condition can be decomposed into simple

structures, which model the environment of the investigated volume. These simple structures permit one to calculate the "responses" beforehand, prior to an iterational procedure.

A specific numerical procedure has been proposed in Section IV. The method provides an interpolating function that satisfies the equation everywhere inside the nodes, and has as many free coefficients as are needed to assure the required continuity condition at node interfaces. The proposed algorithm has been applied in neutron diffusion production codes and which have been employed in the design and operation of nuclear power plants. In a typical problem, the number of nodes is 10^3 - 10^4, the node sizes are in the range of 10-20 cm, the achieved relative accuracy is 10^{-4} in eigenvalue and 1-3%in the power distribution (practically the solution). The results have been compared to the two best known numerical procedures (finite difference and finite element method). A variational formalism has also been given to stress the advantage of using symmetry considerations in the solution of boundary value problems.

VIII. ACKNOWLEDGMENT

The present work had not been prepared without the help of Dr. Yuri Orechwa (ANL), who got the idea, collected a considerable part of the literature and reviewed the manuscript several times. The author is deeply indebted to those who in the numerous opportunities offered by the Temporary International Collective to Study WWER Type Reactors, contributed to the achievements during several years by their remarks or criticism. Special thanks to Drs. András Dévényi, János Gadó, András Kereszturi (KFKI Atomic Energy Research Institute, Budapest), Dr. Lev Maiorov and Dr. Nicolay Laletin (Kurchatov Institute, Moscow).

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APPENDIX A. GROUP THEORY PRIMER

This appendix summarizes the results of group theory applied throughout the present work. The below cited results are available in standard textbooks.

Definition A.1. Let us consider function f(x). The transformation operator associated with operator O is defined by the following identity in x:

$$Of(x) \equiv f(O^{-1}x) \tag{A.1}$$

where O is the matrix associated with operator O.

With this definition the set of symmetry operations (symmetries) is made isomorphic with the set of matrices associated with the symmetries.

Definition A.2. O is called a symmetry of region V if **O** maps V into itself.

Definition A.3. O is called a symmetry of operator **A** if **AO=OA**.

Definition A.4. A set of matrices under matrix multiplication, $\{O_1, O_2, ..., O_n\}$, which is homomorphic with the group $\{O_1, O_2, ...,O_n\}$ is said to be a representation of the group.

Definition A.5. A representation is said to be reducible if an equivalent representation[3] exists in which each matrix O_i has the form

$$\mathbf{O_i} = \begin{pmatrix} \mathbf{A_i} & \mathbf{C_i} \\ 0 & \mathbf{B_i} \end{pmatrix} . \tag{A.2}$$

---

[3]Representations $\{\mathbf{A}_i\}$ and $\{\mathbf{B}_i\}$ are said equivalent if there exists a matrix **X** such that $\mathbf{B}_i=\mathbf{X}\mathbf{A}_i\mathbf{X}^{-1}$ for all i.

If no such a representation exists, the representation is said to be an irreducible representation of the group.

Definition A.6. Let $\{O_i\}$ be an irreducible representation and let $\{f^{(1)}_i, f^{(2)}_i, ..., f^{(l_i)}_i\}$ be l_i eigenfunctions of the symmetry operations for which

$$\mathbf{O} f^{(k)}_i = \sum_{j=1}^{l_i} O_{jk} f^{(j)}_i \qquad \text{(A.3)}$$

holds for $O = O_1, ..., O_h$. A function $f^{(k)}_i$ is said to belong to the k-th row of the irreducible representation O_i if there exist partner functions $\{f^{(1)}_i, f^{(2)}_i, ..., f^{(k-1)}_i, f^{(k+1)}_i, ..., f^{(l_i)}_i\}$ such that the above equation is satisfied.

Shur's Lemma. If there exists a matrix M, not necessarily one of the representation matrices $\{\mathbf{O}_i\}$, such that $\mathbf{MO}_i = \mathbf{O}_i\mathbf{M}$ for all i, then

a. if $\{\mathbf{O}_i\}$ is irreducible, **M** is a constant matrix; that is, $\mathbf{M}=c\mathbf{E}$ where c is a number, **E** is the identity matrix.
b. If **M** is not a constant matrix, then $\{\mathbf{O}_i\}$ is reducible.

Proof: Ref. [13], p.24

Theorem A.1. Any representation of group G is equivalent, by means of a similarity transformation, to a unitary representation.

Proof: Ref. [13], p.22

Theorem A.2. Let S commute with all O_i. Let $f^{(j)}_i$ and $g^{(j')}_{i'}$ belong to different irreducible representations. Then

$$(f_i^{(j)}, g_{i'}^{(j')}) = \frac{1}{j_i} \delta_{ii'} \delta_{jj'} \sum_j (f_i^{(j)}, g_{i'}^{(j')}) \tag{A.4}$$

and

$$(f_i^{(j)}, \mathbf{S} g_{i'}^{(j')}) = \frac{1}{j_i} \delta_{ii'} \delta_{jj'} \sum_j (f_i^{(j)}, \mathbf{S} g_{i'}^{(j')}) . \tag{A.5}$$

Proof: Ref. [49], p. 115-116.

The following theorem, taken from Ref. [13], p. 52-55, is a summary of the relationship between the eigenspace of an operator (in our case **A**) and a group commuting with **A**. The relationship is twofold. The eigenfunctions of **A** may serve as basis functions of the irreducible representations. The symmetry operators on that basis are represented by matrices and the eigenvectors of those matrices are linear combinations of the eigenfunctions of **A**, furthermore, they are basis vectors of an irreducible representation. The reverse statement is: If irreducible functions are used to represent operator **A** by matrices, the resulting matrix will be diagonal, the elements belonging to partner functions of a riven irrep are the same.

Theorem A.3.

1. The eigenfunctions of operator **A** generate a representation of G.
2. Linear transformations to new eigenfunctions generates a representation equivalent to the original.
3. If the eigenfunctions are orthonormal, then operator O is merely the matrix associated with O.
4. The representation so generated is unitary.
5. If the degeneracy is normal, the representation is irreducible.
6. An arbitrary function Φ in the space of **A** can be used to construct an invariant subspace by forming the operation $O\Phi$ for all O in G.
7. Functions which transform according to two different irreducible representations of G are orthogonal.
8. Any function in the space of **A** can be decomposed into a linear combination of functions transforming according to irreps of G.

The operator

$$P^{(i)} \equiv \frac{l_i}{h} \sum_O \chi^{(i)}(O) P_O \tag{A.6}$$

projects out the component transforming according to the ith representation of group G.

Theorem A.4. Let Φ_i be irreducible, i = 1,...,n_c (the number of classes).Then the matrix

$$\langle \Phi_i \mathbf{A} \Phi_j \rangle$$

is diagonal. The elements belonging to the components of a multi (i.e. two or three) dimensional representation are equal.

Proof: this statement is an immediate consequence of the Wigner-Eckart theorem, see Ludwig-Falter, Ref. [25], p. 129-134.

For most point groups, the product of two irreps can be expanded according to the same basis function set as the irreps themselves. The same is true if an operator transforming according to an irrep is applied to a function transforming according to another irrep. Because the dimension of the product is usually larger then the dimension of the components, it may contain a number f irreps. Let $f^{(i1)}{}_{j1}$ and $g^{(i2)}{}_{j2}$ be the basis functions in two irreducible subspaces. Their product will have the form (see Ref.[25], p.84).

$$f_{j1}^{(i1)} g_{j2}^{(i2)} = \sum_{j3,i3} \left(\begin{array}{cc|c} i1 & i2 & i3 \\ j1 & j2 & j3 \end{array} \right) f_{j3}^{(i3)} . \tag{A.7}$$

Here the term in brackets is the Clebsch-Gordan coefficient.

APPENDIX B. BASIC NOTIONS OF NEUTRON DIFFUSION AND TRANSPORT

Appendix B explains the basic notions of neutron diffusion. This may give the reader hint as to the underlying assumptions on the operators and the solutions of the equations.

The elementary solution satisfying the DE

$$-\nabla^2\Phi_j(x) + \mathbf{S}_j\Phi_j(x) = 0 \tag{B.1}$$

in a homogeneous region V_j is

$$\Phi_j(x) = \mathbf{t}_j^{(k)} e^{\lambda_k b x} \tag{B.2}$$

where $|b| = 1$, and $t_j(k)$ denotes the G eigenvectors of the S_j matrix:

$$\mathbf{S}_j\mathbf{t}_j^{(k)} = \lambda_k^2\mathbf{t}_j^{(k)}. \tag{B.3}$$

The matrix S_j is often expressed (dropping the volume index j) as $\mathbf{S}_j = \lambda\mathbf{P}\text{-}\mathbf{D}$, where **P** is the production, **D** is the destruction operator. The elements of matrix S are

$$S_{gg'} = \Sigma_g - \frac{\chi_g}{k}\nu\Sigma_{fg'} - \Sigma_{sg'\to g}.$$

Another notation is $\mathbf{S}_i=\mathbf{P}/k_{eff}\text{-}\mathbf{D}$. The value of λ (or k_{eff}), at which the homogeneous problem has a nontrivial solution, is called critical eigenvalue. Note that k_{eff} pertains to volume V and not to any of V_i subvolumes. The power distribution is

$$P_j = \frac{1}{V_j}\int_{V_j}\left(\Phi_{j1}\Sigma_{f1} + \Phi_{j2}\Sigma_{f2}\right)dV_j \tag{B.4}$$

where Φ_{ji} stands for the flux in volume V_j, in energy group i. The cross-sections are given in each subvolume.

In the neutron transport equation (TE), the angular flux $\Phi(x,E,\Omega)$ is the dependent variable. It gives the the distance travelled by the neutrons located at x, having energy E and flying direction Ω. The transport equation reads as

$$(-\Omega\nabla + \Sigma(x,E))\Phi(x,E,\Omega) = \int\int \Sigma_s(x;E',\Omega',E,\Omega)\Phi(x,E',\Omega')dE'd\Omega' + Q(x,E,\Omega) . \tag{B.5}$$

Where Q contains the source. When no external source is present, Q is the fission source:

$$Q(x,E,\Omega) = \frac{1}{4\pi}\frac{\chi(E)}{k_{eff}} \int\int \nu\Sigma_f(x,E')\Phi(x,E',\Omega')dE'd\Omega' .$$

The partial currents are given by

$$I^{\pm}(x,E) = \int_{\Omega n><0} \mathbf{n}\Omega\Phi(x,E,\Omega)d\Omega \tag{B.6}$$

where n is the outward normal at position x. The angular flux is often expressed in terms of the first few lower order Legendre or spherical harmonics components. Such an expression may be

$$\Phi(x,E,\Omega) = \frac{1}{4\pi}\int\Phi(x,E,\Omega)d\Omega + \frac{3}{4\pi}\int\Omega\Phi(x,E,\Omega)d\Omega \tag{B.7}$$

where the first term is the so called scalar flux, the second term is the net current.

Distribution:

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